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Data article

Title:

FABP4 inhibitors 3D-QSAR model and isosteric replacement of BMS309403 datasets

Authors:

Giuseppe Floresta[a,b,c,*], Agostino Cilibrizzi[c,d], Vincenzo Abbate[d], Ambra Spampinato[a], Chiara Zagni[a], Antonio Rescifina[a,*]

Affiliations:

[a] Department of Drug Sciences, University of Catania, V.le A. Doria 6, 95125 Catania, Italy

[b] Department of Chemical Sciences, University of Catania, V.le A. Doria, 95125 Catania, Italy

[c] Institute of Pharmaceutical Science, King's College London, Stamford Street, London SE1 9NH, UK

[d] King's Forensics, School of Population Health & Environmental Sciences, King's College London, Franklin-Wilkins Building, 150 Stamford Street, London SE1 9NH

Contact email:

giuseppe.floresta@unict.it (G. Floresta) and arescifina@unict.it (A. Rescifina)

Abstract

The data have been obtained from FABP4 inhibitor molecules previously published. The 120 compounds were used to build a 3D-QSAR model. The development of the QSAR model has been undertaken with the use of Forge software using the PM3 optimized structure and the experimental IC_{50} of each compound. The QSAR model was also employed to predict the activity of 3000 new isosteric derivatives of BMS309403. The isosteric replacement was also validated by the synthesis and the biological screening of three new compounds reported in the related research article "3D-QSAR assisted identification of FABP4 inhibitors: An effective scaffold hopping analysis/QSAR evaluation"[1].

Specifications Table

Subject area	*Computational Chemistry*

More specific subject area	*Three-Dimensional Quantitative Structure-Activity Relationship (3D-QSAR) modeling*
Type of data	*Tables, figures*
How data was acquired	*Statistical modeling and online databases*
Data format	*Raw and analyzed*
Experimental factors	*The whole dataset consists of 120 FABP4 ligands and 3000 isosteric derivatives of BMS309403*
Experimental features	*The 3D-QSAR model has been developed using Forge as software. Chemical structure descriptors and pIC_{50} were used as variables. Spark was used for the isosteric replacement*
Data source location	*Department of Drug Sciences, University of Catania, Italy*
Data accessibility	*Data is with this article*
Related research article	G. Floresta, A. Cilibrizzi, V. Abbate, A. Spampinato, C. Zagni, A. Rescifina, 3D-QSAR assisted identification of FABP4 inhibitors: An effective scaffold hopping analysis/QSAR evaluation, Bioorganic Chemistry, 84 (2019) 276-284 [1].

Value of the data

- FABP4 recently demonstrated an interesting molecular target for the treatment of type 2 diabetes, other metabolic diseases and some type of cancers.
- QSAR modeling data was generated to provide a method useful in finding or repurposing novel FABP4 ligands.
- The model has also been used to predict the activity of 3000 isosteric derivatives of BMS309403.
- The data can be used by others to build their own model.
- The data can be used for the synthesis of some potent suggested compounds.

Data

FABP4 recently demonstrated an interesting molecular target for the treatment of type 2 diabetes, other metabolic diseases and some type of cancers [2-10]. Recently, a variety of effective FABP4 inhibitors have been developed [11], but unfortunately, none of them is currently in the clinical research phases. CAMD shows a promising and effective tool for the identification of FABP4 inhibitors [12-15]. In line with our recent interest in the development of QSAR models and related applications [16-24], in order to identify novel hit compounds, herein we report the dataset and the parameter used to build a 3D-QSAR model for FABP4. This dataset is reported in Tables 2 and 3, were the molecules used in the training set (96) and in the test set (24) are reported, respectively. Information for the building of the 3D-QSAR model is reported in Figures 1–9. Moreover, the 3D-QSAR model was also used to predict the biological activity of 3000 new isosteric derivatives of BMS309403 derived from a scaffold-hopping analysis, the analyzed areas of the selected compounds and the Spark's parameters used for the isosteric replacement are reported in Figures 8 and 9. The results of the isosteric replacement of different portion of BMS309403 are reported in Tables 4–9.

Experimental Design, Materials and Methods

Compounds alignments

With the aim to generate a plausible and consistent set of alignment molecules, before running the regression analysis, we evaluated two different types of alignment (Fig. 1).

First, we evaluated a structure-based alignment, based on the docking of the different ligands on the active site of the protein. All 120 structures, optimized at the PM3 level of theory [25-27], have been converted into pdbqt format using Babel,[28] and subsequently docked in the active site of FABP4. Molecular docking was performed using the three-dimensional crystal structures of substrate-free fatty acid binding protein 4 in complex with BMS309403 (PDB ID: 2NNQ) obtained from the Protein Data Bank (PDB, http://www.rcsb.org/pdb). AutoDock Vina (version 1.1.2)[29], was used for all docking experiments. The default values of the docking parameters in AutoDock Vina were all maintained, except for "exhaustiveness" that was set to 15. A grid box of 18 Å × 18 Å × 18 Å was used, encompassing the inhibitor binding cavity of FABP4 and centered on the ligand. The binding modes were clustered through the root mean square deviation among the Cartesian coordinates of the ligand atoms. The docking results were ranked based on the binding free energy. After the calculations with AutoDock Vina, all the generated structures were manually checked, in order to ensure a correct positioning within the binding site. Then the generated structures were imported into Forge [30] to build the Structure-based 3D-QSAR model. A classic ligand-based alignment is the second type of alignment that was evaluated. This was carried out with the same software used for the building of the model. All the optimized structures, together with their respective IC_{50} values, were imported into Forge (10.4.2, Cresset, Litlington, Cambridgeshire, UK, http://www.cresset-group.com/forge) [30-34] for setting-up the field-based 3D-QSAR model. Eight different molecules were chosen as a template for the calculations of field points and as a template for the alignment. These eight molecules were selected since they are present in crystallized forms with FABP4 (PDB IDs: 2NNQ, 3FR2, 3FR4, 3FR5, 4NNS, 4NNT, 1TOU and 1TOW, Table 1) [35-38]. The structures, small protein, and inhibitors, were first downloaded from the Protein Data Bank (PDB); the amino acid sequence was then superposed and aligned with YASARA (version 17.8.15) to get also the ligands in the binding site aligned and superposed, thus the eight molecules were imported on Forge (Fig. 2 and 3).

The XED (eXtended Electron Distribution) force field was used to generate the field point .The compounds in the training set were aligned to the reference compound by maximum common substructure using a customized set-up for the conformation hunt:

- Max number of conformations: 500.
- RMS cut-off for duplicate conformers: 0.5 Å.
- Gradient cut-off for conformer minimization: 0.1 kcal/mol.
- Energy window: 2.5 kcal/mol.

The RMS cut-off for duplicate conformers parameter controls the similarity threshold below which two conformers are assumed identical. Conformations that gave a minimized energy outside the energy window were discarded.

All the alignments were manually checked to ensure the best possible model. All the field points of the training set were used to derive a gauge invariant set of sampling points, which reduced the number of descriptors that needed to be taken into account, with a distance of 1 Å between the sample points.

Sample values were calculated, ensuring that all areas around the molecule (and possibly contributing to the activity) are properly described.

Statistical analysis

For the validation of the QSAR model, the leave-one-out method was used. 20 was the maximum number of components to extract from the PLS regression. 50 was the number of Y scrambles to use The threshold of the sample point minimum distance was set to 1 Å. The Leave-one-out method was used during the validation of the QSAR model.. The regression method used in Forge was PLS (SIMPLS algorithm) [39-43]. All the parameters for the QSAR model are resumed in Figures 4–6.
The predictive ability of the generated QSAR model was confirmed by several statistical tests. The cross-validation regression coefficient (q^2) was calculated based on the PRESS (Prediction error sum of squares) and SSY (Sum of squares of deviation of the experimental values from their mean):

$$q^2 = 1 - \frac{PRESS}{SSY} = 1 - \frac{\sum_{i=1}^{n}(Yexp - Ypred)^2}{\sum_{i=1}^{n}(Yexp - Ymean)^2}$$

Y*exp* = experimental activity of training set compound
Y*pred* = predicted activity of training set compound
Y*mean* = mean values of the activity of training set compound

The derived ligand-based approach results to be more reliable (r^2 = 0.92, q^2 = 0.64) than the structure-based alignment (r^2 = 0.90, q^2 = 0.38). The ligand-based 3D-QSAR align model was further validated with a set of external compounds (*i.e*. test set). Out of 120 molecules, we randomly choose 96 molecules (covering the whole range of activities of the compounds) as a training set to build the model, while the remaining 24 compounds served as a test set to evaluate the model.
The statistical reliability of this model was also validated by the determination of the r^2test, using the following equation:

$$r^2test = 1 - \frac{\sum_{i=1}^{n}(Ypredtest - Ytest)^2}{\sum_{i=1}^{n}(Ytest - Ymean)^2}$$

Y*predtest* = predicted activity of test set compound by QSAR equation
Y*test* = experimental activity of test set compound
Y*mean* = mean values of the activity of training set compound

The 11-components model (Fig. 7) shows both good predictive and descriptive capability as it is shown by the good r^2 (0.99) and q^2 (0.69) [44] values for the training and the cross-validated training sets. The plot of experimental *vs*. predicted activity for the compounds, in both the training set and the cross-validated training set (q^2 = 0.69), shows a reasonable distribution of the values. The plot of experimental *vs*. predicted activity for the compounds in the test set is still reasonably good with only few outliers and a good cross-validated r^2 of 0.73.

Isosteric replacement

The isosteric replacement was performed using Spark as a software (10.4.0, Cresset, Litlington, Cambridgeshire, UK, http://www.cresset-group.com/forge) [30-34]. As reported in Fig. 8, Different portions of the BMS309403 were replaced. Then, the newly designed molecules were aligned with the 3D-QSAR model and evaluated. The replacement was performed through the same 178,558 fragments for each part, which derive from ChEMBL and Zinc databases (Fig. 9) [45, 46]. Five hundred compounds were generated for each substitution producing 3,000 hits (reported in Tables 4–9). There of the suggested molecules were synthesized and tested as reported in the related research article [1].

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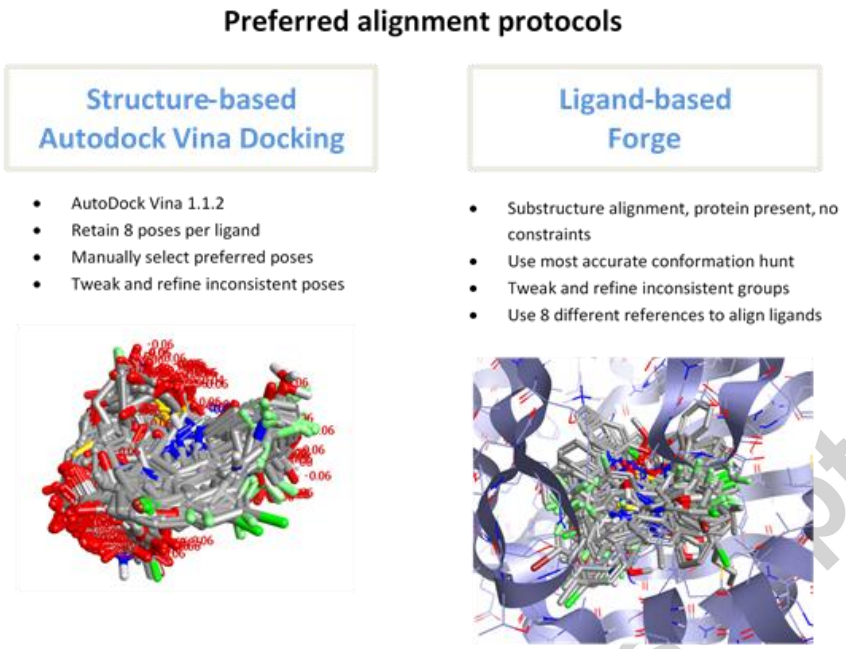


Fig. 1. Comparison of alignment methods.

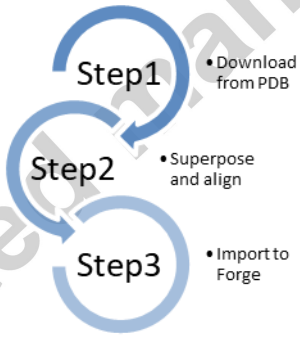
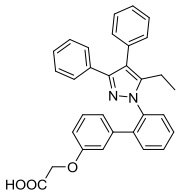
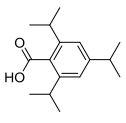
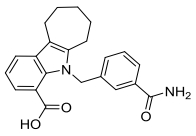
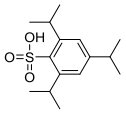
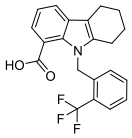
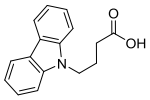
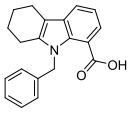
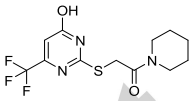


Fig. 2. Schematic representation of the process adopted to obtain the template compounds for the ligand-based alignment.

Table 1

PDB codes and molecules used as reference compounds for ligand-based alignment.

PDB code	2D structure	PDB code	2D structure
2NNQ		4NNT	

3FR5		4NNS	
3FR4		1TOW	
3FR2		1TOU	

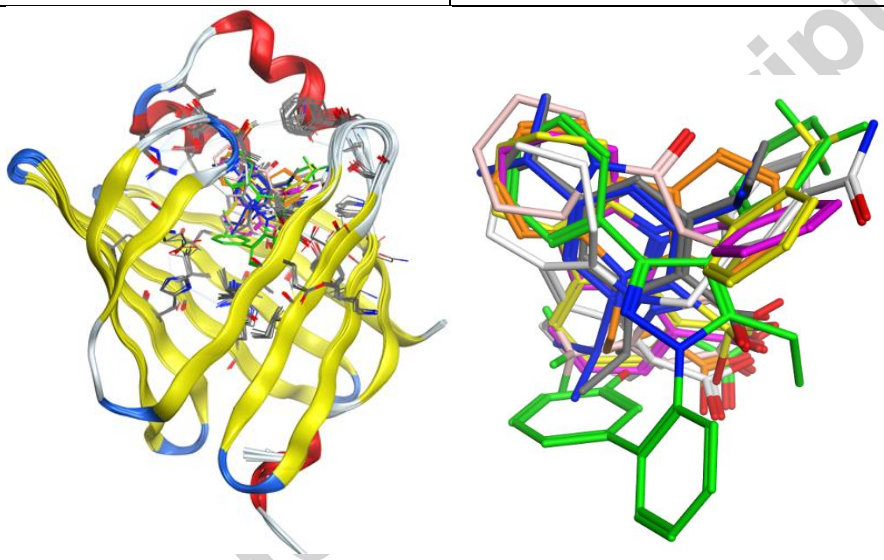


Fig. 3. A) Protein and inhibitors aligned. B) Aligned inhibitors imported to Forge for ligand-based alignment.

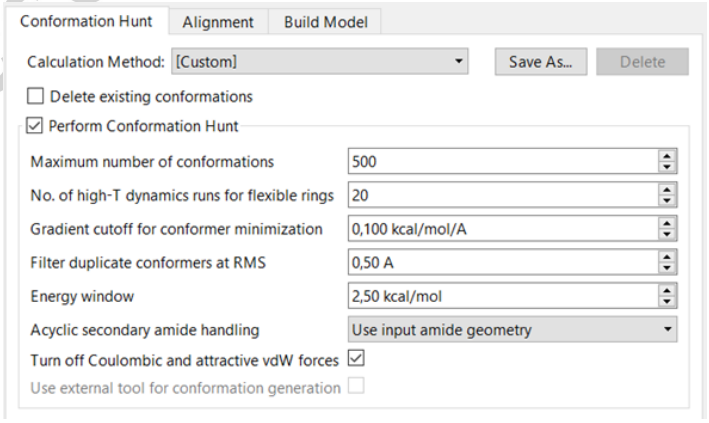


Fig. 4. Forge's parameters used for conformation hunt.

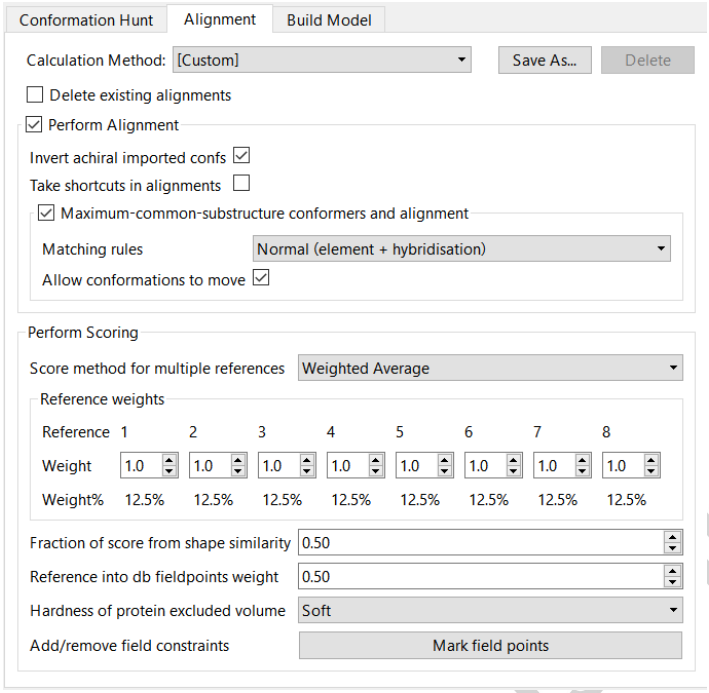


Fig. 5. Forge's parameters used for alignment.

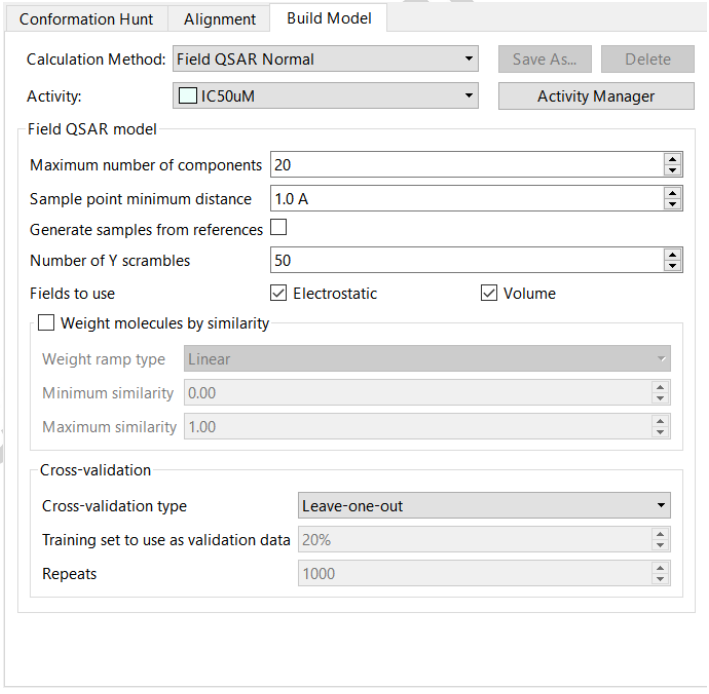


Fig. 6. Forge's parameters used to build the QSAR model.

Model statistics:
==========

Comps	R^2	Q^2	Test R^2	RMSE	RMSEpred	Tau	Tau-pred
0	-0.044	-0.023	-0.001	1.093	1.096	0.494	-0.910
1	0.620	0.508	0.641	0.666	0.767	0.587	0.492
2	0.781	0.541	0.625	0.501	0.740	0.675	0.514
3	0.897	0.585	0.718	0.347	0.711	0.787	0.573
4	0.948	0.618	0.745	0.244	0.681	0.855	0.568
5	0.968	0.636	0.743	0.192	0.663	0.895	0.598
6	0.983	0.651	0.772	0.142	0.651	0.920	0.594
7	0.988	0.671	0.746	0.118	0.631	0.929	0.621
8	0.993	0.673	0.757	0.088	0.629	0.947	0.621
9	0.996	0.683	0.744	0.068	0.619	0.958	0.633
10	0.997	0.687	0.733	0.058	0.616	0.957	0.626
11*	0.998	0.688	0.731	0.044	0.615	0.969	0.626
12	0.999	0.683	0.729	0.037	0.619	0.969	0.618
13	0.999	0.680	0.726	0.030	0.622	0.976	0.616
14	1.000	0.679	0.731	0.022	0.623	0.983	0.613
15	1.000	0.679	0.730	0.018	0.623	0.985	0.615
16	1.000	0.678	0.728	0.015	0.624	0.988	0.616
17	1.000	0.678	0.728	0.011	0.625	0.988	0.615
18	1.000	0.677	0.730	0.008	0.625	0.991	0.615
19	1.000	0.678	0.728	0.006	0.625	0.993	0.616
20	1.000	0.677	0.728	0.005	0.625	0.995	0.616

Preferred number of components: 11

Fig. 7. Model statistics for FABP4 model.

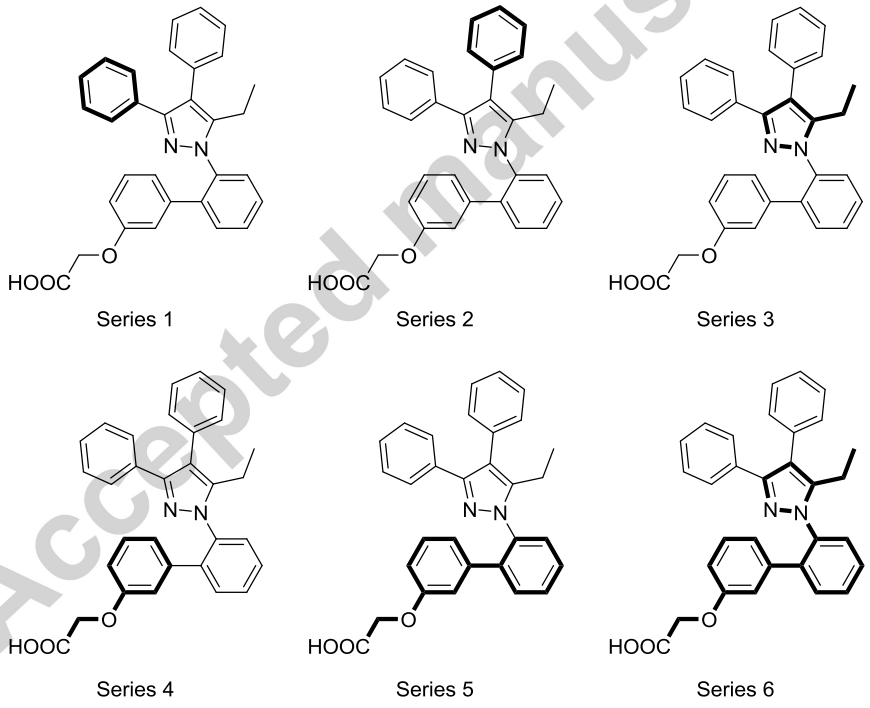


Fig. 8. The studied position for the bioisosteric replacement of BMS309403 are highlighted in bold.

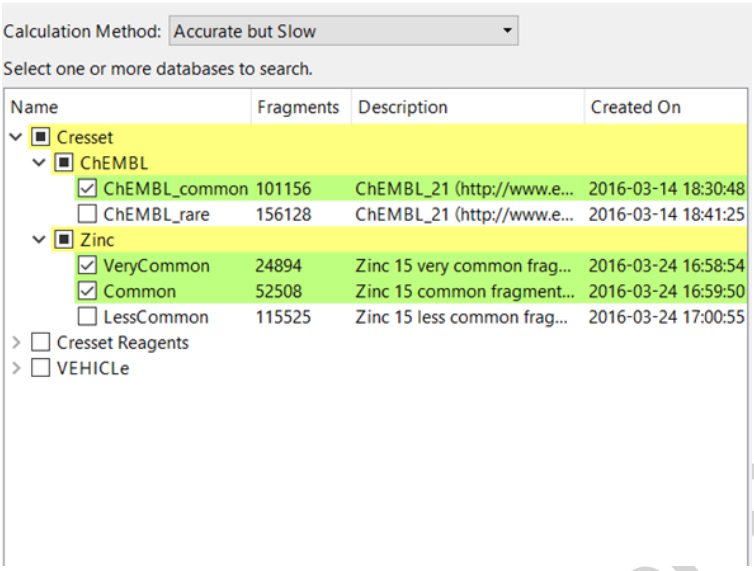


Fig. 9. Spark's parameters used for bio-isosteric replacement.

Table 2

SMILES, experimental and predicted pIC_{50} values of the molecules in the training set.

		pIC_{50}	
N°	**SMILES**	**Exp.**	**Pred.**
1	FC(F)(F)[C@H]1CCc2c(C1)c(c(c(n2)C3CCCC3)C=4[N-]N=NN4)-c5ccnc(c5)C	8.0	8.0
2	CC1(CCCC1)c2c(c(c3c(n2)CCCCC3)-c4ccnc(c4)C)C=5[N-]N=NN5	8.0	8.0
3	Clc1c(F)cc2c(c(c(c(N(CC)CC)n2)C=3[N-]N=NN3)-c4ccccc4)c1	7.9	7.9
4	Clc1c(F)cc2c(c(c(c(n2)C(CC)CC)C=3[N-]N=NN3)-c4ccccc4)c1	7.8	7.8
5	OCC1(CCCC1)c2c(c(c3c(n2)CCCCC3)-c4ccnc(c4)C)C=5[N-]N=NN5	7.7	7.7
6	CCCCC[C@H]1CCc2c(C1)c(c(c(n2)C3(CCCC3)COC)C=4[N-]N=NN4)-c5ccccc5	7.7	7.7
7	FC(F)(F)c1ccc2c(c(c(c(N3CCCCC3)n2)C=4[N-]N=NN4)-c5ccccc5)c1	7.5	7.5
8	Clc1ccc2c(c(c(c(n2)C3CC3)C([O-])=O)-c4ccccc4)c1	7.4	7.4
9	Clc1ccc2c(c(c(c(N(CC)C)n2)C=3[N-]N=NN3)-c4ccccc4)c1	7.3	7.4
10	Clc1cc(Cl)cc(NC(=O)NC2(CCCC2)C([O-])=O)c1-c3ccccc3	7.3	7.3
11	Clc1c(F)cc(c(NC(=O)NC2(CCCC2)C([O-])=O)c1)-c3ccccc3	7.0	7.0
12	O=C(N)c1ccccc1Cn2c3c(cccc3c4CCCCCc42)C([O-])=O	7.0	7.0
13	n1c2c(CCCCC2)c(c(c1C3CCCCC3)C=4[N-]N=NN4)-c5ccncc5	7.0	6.9
14	Clc1ccc(c(NC(=O)NC2(CCCC2)C([O-])=O)c1)-c3ccc(F)cc3	6.9	6.9
15	FC(F)(F)c1ccccc1Cn2c3c(cccc3c4CCCCc42)C([O-])=O	6.4	6.5
16	Fc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1	6.5	6.5
17	[O-]C(=O)c1cccc2c3CCCCCc3n(c12)Cc4ccccc4	6.2	6.3
18	Fc1ccccc1Cn2c3c(cccc3c4CCCCc42)C([O-])=O	6.4	6.3
19	Fc1cccc(Cn2c3c(cccc3c4CCCCc42)C([O-])=O)c1	6.4	6.3

20	FC(F)(F)c1ccccc1Cn2c3c(cccc3c4CCCCCc42)C([O-])=O	6.2	6.3
21	[O-]C(=O)CCCn1c2ccccc2c3ccccc31	6.2	6.3
22	FC(F)(F)c1ccc(c(NC(=O)NC2(CCCC2)C([O-])=O)c1)-c3ccccc3	6.3	6.2
23	[O-]C(=O)c1cccc2c3CCCCc3n(c12)Cc4cccc(OC)c4	6.3	6.2
24	Fc1cccc(Cn2c3c(cccc3c4CCCCCc42)C([O-])=O)c1	6.1	6.2
25	FC(F)(F)c1cc(O)nc(SCc2ccc(OC)cc2)n1	6.2	6.2
26	[O-]C(=O)c1ccc2c(n(c3CCCCc23)Cc4ccccc4)c1	6.1	6.1
27	[O-]C(=O)c1cccc2c3CCCc3n(c12)Cc4ccccc4	6.1	6.1
28	[O-]C(=O)c1cccc2c3CCCCc3n(c12)Cc4ccccc4OC	6.2	6.1
29	[O-]C(=O)c1cccc2c3CCCCc3n(c12)Cc4ccc(C)cc4	6.0	6.1
30	Fc1ccccc1Cn2c3c(cccc3c4CCCCCc42)C([O-])=O	6.2	6.1
31	Fc1ccc(Cn2c3c(cccc3c4CCCCCc42)C([O-])=O)cc1	6.1	6.1
32	[O-]C(=O)CCCCn1c2ccccc2c3ccccc31	6.1	6.1
33	FC(F)(F)c1cccc(Cn2c3c(cccc3c4CCCCCc42)C([O-])=O)c1	6.0	6.0
34	FC(F)(F)c1cc(O)nc(SCC(=O)N2CCCCC2)n1	6.0	6.0
35	O=S(=O)(n1ccc2ccc(cc21)C)c3ccsc3C([O-])=O	5.9	5.9
36	Brc1ccc2c(ccn2S(=O)(=O)c3ccsc3C([O-])=O)c1	5.9	5.9
37	FC(F)(F)c1cccc(Cn2c3c(cccc3c4CCCCc42)C([O-])=O)c1	5.8	5.7
38	FC(F)(F)c1ccc(Cn2c3c(cccc3c4CCCCc42)C([O-])=O)cc1	5.6	5.7
39	FC(F)(F)c1ccc(Cn2c3c(cccc3c4CCCCCc42)C([O-])=O)cc1	5.7	5.7
40	O=S(=O)(n1cc(c2ccccc21)C)c3ccsc3C([O-])=O	5.8	5.7
41	[O-]C(=O)c1cccc2c3CCCCc3n(c12)Cc4ccc(OC)cc4	5.6	5.6
42	[O-]C(=O)[C@H](Oc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.6	5.6
43	O=S(=O)(n1ccc2cccc(OC)c21)c3ccsc3C([O-])=O	5.6	5.6
44	O/N=C/1CCCc2c1c3cccc(c3n2Cc4ccccc4)C([O-])=O	5.5	5.5
45	Clc1cccc(-n2c(-c3ccccc3)cc(n2)-c4ccccc4OCCCC([O-])=O)c1	5.6	5.5
46	[O-]C(=O)[C@H](Oc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC	5.5	5.5
47	Fc1ccc2c(ccn2S(=O)(=O)c3ccsc3C([O-])=O)c1	5.5	5.5
48	[O-]C(=O)c1cccc2c(c(n(c12)Cc3ccccc3)C)C	5.4	5.4
49	Clc1ccc(-n2c(-c3ccccc3)cc(n2)-c4ccccc4OCCCC([O-])=O)cc1	5.4	5.4
50	Clc1ccccc1-n2c(-c3ccccc3)cc(n2)-c4ccccc4OCCCC([O-])=O	5.4	5.4
51	[O-]C(=O)c1c(C(C)C)cc(C(C)C)cc1C(C)C	5.4	5.4
52	O=S(=O)(n1c2ccccc2c3ccccc31)c4ccccc4C([O-])=O	5.4	5.4
53	Fc1ccc2ccn(S(=O)(=O)c3ccsc3C([O-])=O)c2c1	5.4	5.4
54	FC(F)(F)c1cc(O)nc(NCc2ccc(OC)cc2)n1	5.4	5.4
55	[O-]C(=O)CCCOc1ccccc1-c2cc(n(n2)-c3ccccc3)-c4ccc(cc4)C	5.3	5.3
56	Brc1ccc(-n2c(-c3ccccc3)cc(n2)-c4ccccc4OCCCC([O-])=O)cc1	5.3	5.3
57	Fc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.3	5.3
58	[O-]C(=O)CCCCOc1ccccc1-c2cc(n(n2)-c3ccccc3)-c4ccccc4	5.2	5.2
59	O=S(=O)(n1ccc2cc(ccc21)C)c3ccsc3C([O-])=O	5.2	5.2
60	O=S(=O)(n1ccc2ccc(OC)cc21)c3ccccc3C([O-])=O	5.2	5.2
61	Brc1ccc(-c2cc(nn2-c3ccccc3)-c4ccccc4OCCCC([O-])=O)cc1	5.0	5.0
62	Fc1ccc(-n2c(-c3ccccc3)cc(n2)-c4ccccc4OCCCC([O-])=O)cc1	5.0	5.0
63	[O-]C(=O)CCCOc1ccccc1-c2cc(n(n2)-c3ccc(C(C)C)cc3)-c4ccccc4	5.0	5.0
64	[O-]C(=O)CCn1c2ccccc2c3ccccc31	5.0	5.0

65	O=S(=O)(n1ccc2c(cccc21)C)c3ccsc3C([O-])=O	5.1	5.0
66	O=S(=O)(n1ccc2cc(OC)ccc21)c3ccsc3C([O-])=O	5.1	5.0
67	O=S(=O)(n1cc(c2ccccc21)C)c3ccccc3C([O-])=O	5.1	5.0
68	O=S(=O)(n1ccc2c(cccc21)C)c3ccccc3C([O-])=O	4.9	4.9
69	Brc1ccc2c(ccn2S(=O)(=O)c3ccccc3C([O-])=O)c1	4.9	4.9
70	[O-]C(=O)CCCOc1ccccc1-c2cc(n(n2)-c3ccc(OC)cc3)-c4ccccc4	4.9	4.8
71	[O-]C(=O)CCCOc1ccccc1-c2cc(n(n2)C3CCCCCC3)-c4ccccc4	4.8	4.8
72	Brc1ccc2c(n(S(=O)(=O)c3c(C(C)C)cc(C(C)C)cc3C(C)C)cn2)c1	4.8	4.8
73	Clc1ccc2c(nc(n2S(=O)(=O)c3c(C(C)C)cc(C(C)C)cc3C(C)C)C)c1	4.8	4.8
74	O=S(=O)(n1cncc1)c2c(C(C)C)cc(C(C)C)cc2C(C)C	4.7	4.8
75	Clc1ccccc1CNc2nc(O)cc(n2)C(F)(F)F	4.6	4.7
76	FC(F)(F)c1cc(O)nc(n1)CCc2ccc(OC)cc2	4.6	4.7
77	O=C1CCCc2c1c3cccc(c3n2Cc4ccccc4)C([O-])=O	4.6	4.6
78	[O-]C(=O)CCCOc1ccccc1-c2cc(n(n2)C3CCCCC3)-c4ccccc4	4.6	4.6
79	O=S(=O)(n1ccc2cc(ccc21)C)c3ccccc3C([O-])=O	4.5	4.6
80	FC(F)(F)c1cc(O)nc(n1)N(Cc2ccccc2)C	4.6	4.6
81	Clc1ccc(-c2cc(nn2-c3ccccc3)-c4ccccc4OCCCCCCC([O-])=O)cc1	4.5	4.5
82	FC(F)(F)c1cc(O)nc(NCC(=O)N2CCCCC2)n1	4.4	4.4
83	Clc1cccc(CNc2nc(O)cc(n2)C(F)(F)F)c1	4.5	4.4
84	FC(F)(F)c1cc(O)nc(NCc2ccc(C)cc2)n1	4.5	4.4
85	Clc1ccc(-c2cc(nn2-c3ccccc3)-c4ccccc4OCCCCC([O-])=O)cc1	4.1	4.2
86	Brc1ccc(-c2cc(nn2-c3ccccc3)-c4ccccc4OCCCCC([O-])=O)cc1	4.1	4.1
87	O=S(=O)(n1ccc2c(OC)cccc21)c3ccccc3C([O-])=O	4.1	4.1
88	O=S(=O)(N)c1c(C(C)C)cc(C(C)C)cc1C(C)C	4.0	4.0
89	[O-]C(=O)Cn1c2ccccc2c3ccccc31	4.0	4.0
90	FC(F)(F)c1cc(O)nc(n1)NCc2ccc(-c3ccccc3)cc2	4.0	4.0
91	FC(F)(F)c1cc(O)nc(NCc2ccncc2)n1	4.0	4.0
92	FC(F)(F)c1cc(O)nc(n1)CCc2ccccc2	4.0	4.0
93	FC(F)(F)c1cc(O)nc(NCCc2ccccc2)n1	4.0	3.9
94	[O-]C(=O)CCCCOc1ccccc1-c2cc(n(n2)-c3ccccc3)-c4ccc(cc4)C	3.6	3.6
95	Clc1ccc(CNc2nc(O)cc(n2)C(F)(F)F)cc1	5.5	3.5
96	Clc1ccc(-c2cc(nn2-c3ccccc3)-c4ccccc4OCC([O-])=O)cc1	2.0	2.0

Table 3

SMILES, experimental, and predicted pIC_{50} values of the molecules in the test set.

		pIC_{50}	
N°	**SMILES**	**Exp.**	**Pred.**
1	FC(F)(F)c1ccc2c(c(c(c(N(CC)CC)n2)C=3[N-]N=NN3)-c4ccccc4)c1	7.6	7.8
2	Clc1c(F)cc2c(c(c(c(N3CCCCC3)n2)C=4[N-]N=NN4)-c5ccccc5)c1	7.9	7.3
3	Clc1ccc(c(NC(=O)NC2(CCCC2)C([O-])=O)c1)-c3ccccc3	6.8	6.5
4	O=C(N)c1cccc(Cn2c3c(cccc3c4CCCCCc42)C([O-])=O)c1	7.2	6.2
5	[O-]C(=O)c1ccc2c(c3CCCCc3n2Cc4ccccc4)c1	4.6	6.1

6	Fc1ccc(Cn2c3c(cccc3c4CCCCc42)C([O-])=O)cc1	6.1	6.1
7	[O-]C(=O)c1cccc2c3CCCCc3n(c12)Cc4ccccc4	6.2	5.9
8	Fc1cccc(c1Cn2c3c(cccc3c4CCCCc42)C([O-])=O)C(F)(F)F	5.7	5.9
9	O=S(=O)(n1c2ccccc2c3ccccc31)c4ccsc4C([O-])=O	6.0	5.9
10	[O-]C(=O)c1cccc2c3CCCCCc3n(CCC)c12	6.4	5.7
11	[O-]S(=O)(=O)c1c(C(C)C)cc(C(C)C)cc1C(C)C	5.1	5.7
12	O=S(=O)(n1ccc2ccc(OC)cc21)c3ccsc3C([O-])=O	5.6	5.7
13	[O-]C(=O)c1cccc2c3CCCCc3n(CCC)c12	6.1	5.6
14	Fc1cccc2ccn(S(=O)(=O)c3ccsc3C([O-])=O)c12	5.4	5.4
15	[O-]C(=O)CCCOc1ccccc1-c2cc(n(n2)-c3ccccc3)-c4ccccc4	5.5	5.3
16	Clc1ccc(-c2cc(nn2-c3ccccc3)-c4ccccc4OCCCC([O-])=O)cc1	5.2	5.2
17	Fc1cccc2c1ccn2S(=O)(=O)c3ccccc3C([O-])=O	5.0	5.2
18	Clc1ccc(CN(c2nc(O)cc(n2)C(F)(F)F)C)cc1	5.4	5.1
19	FC(F)(F)c1cc(O)nc(Nc2ccccc2)n1	4.0	4.8
20	Brc1ccc2c(n(S(=O)(=O)c3c(C(C)C)cc(C(C)C)cc3C(C)C)c(n2)C)c1	4.1	4.7
21	O=S(=O)(n1c(nc2ccccc21)C)c3c(C(C)C)cc(C(C)C)cc3C(C)C	4.0	4.6
22	[O-]C(=O)CCCOc1ccccc1-c2cc(n(n2)C3CCCC3)-c4ccccc4	4.8	4.5
23	O=S(=O)(n1ccc2c(OC)cccc21)c3ccsc3C([O-])=O	4.9	4.3
24	FC(F)(F)c1cc(O)nc(n1)NCc2ccccc2	4.5	4.2

Table 4

SMILE and predicted pIC_{50} values for Series 1 derivatives.

N°	SMILES	$_{Pred}pIC_{50}$
1	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4c(c(c(s4)C)C)C)-c5ccccc5)CC)c1	6.1
2	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4CCCCCC4)-c5ccccc5)CC)c1	6.0
3	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cn(c(c4)C)C)-c5ccccc5)CC)c1	6.0
4	Clc1ccc(O)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	6.0
5	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc5c(s4)ccs5)-c6ccccc6)CC)c1	5.9
6	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(occ5C)c4)-c6ccccc6)CC)c1	5.9
7	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(c(CC)c4)C)-c5ccccc5)CC)c1	5.9
8	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(NC)cc4)-c5ccccc5)CC)c1	5.9
9	Clc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1O	5.9
10	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4c(cc(s4)C)C)-c5ccccc5)CC)c1	5.9
11	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc5cc[nH]c5s4)-c6ccccc6)CC)c1	5.9
12	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc5COCCc5s4)-c6ccccc6)CC)c1	5.9
13	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(c(c[nH]5)C)c4)-c6ccccc6)CC)c1	5.8
14	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(s4)NC)-c5ccccc5)CC)c1	5.8
15	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(N)c4N)-c5ccccc5)CC)c1	5.8
16	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc([nH]4)C)-c5ccccc5)CC)c1	5.8
17	Oc1c(cc(cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C)C	5.8
18	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cnc(OC)c(c4)C)-c5ccccc5)CC)c1	5.8
19	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(N)c4)-c5ccccc5)CC)c1	5.8
20	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(oc4)C)-c5ccccc5)CC)c1	5.8

21	Clc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1N	5.8
22	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(c4N)C)-c5ccccc5)CC)c1	5.8
23	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(C5CC5)c4)-c6ccccc6)CC)c1	5.8
24	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(N)c(N)c4)-c5ccccc5)CC)c1	5.8
25	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc([nH]c4)C)-c5ccccc5)CC)c1	5.8
26	Clc1cc(F)c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1O	5.8
27	Clc1cc(OC)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.8
28	Fc1ccc(N)c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.8
29	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(SC)c4)-c5ccccc5)CC)c1	5.8
30	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(sc4N)C)-c5ccccc5)CC)c1	5.8
31	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc5c([nH]4)ccs5)-c6ccccc6)CC)c1	5.8
32	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc5ccoc5s4)-c6ccccc6)CC)c1	5.8
33	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(N)c(OC)c4)-c5ccccc5)CC)c1	5.8
34	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(n[nH]n5)c4)-c6ccccc6)CC)c1	5.8
35	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(N4CCC(CC4)C)n3)-c5ccccc5)CC)c1	5.8
36	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5cc[nH]c5c4)-c6ccccc6)CC)c1	5.8
37	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(c(c4)C)C)-c5ccccc5)CC)c1	5.7
38	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=CCc5ccccc54)-c6ccccc6)CC)c1	5.7
39	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(NCC)cc4)-c5ccccc5)CC)c1	5.7
40	Oc1c(CC)cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.7
41	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(OCC5)c4)-c6ccccc6)CC)c1	5.7
42	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(NC)c(c4)C)-c5ccccc5)CC)c1	5.7
43	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4ccs5)-c6ccccc6)CC)c1	5.7
44	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(CCCC5)c4)-c6ccccc6)CC)c1	5.7
45	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4c5c(OCCO5)cs4)-c6ccccc6)CC)c1	5.7
46	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(N)c[nH]4)-c5ccccc5)CC)c1	5.7
47	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(cc4)C)-c5ccccc5)CC)c1	5.7
48	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(cc4N)C)-c5ccccc5)CC)c1	5.7
49	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4csc(N)c4)-c5ccccc5)CC)c1	5.7
50	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(ocn5)c4)-c6ccccc6)CC)c1	5.7
51	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(NN)cc4)-c5ccccc5)CC)c1	5.7
52	Oc1ccc(O)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.7
53	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(CCN5)c4)-c6ccccc6)CC)c1	5.7
54	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(N)cs4)-c5ccccc5)CC)c1	5.7
55	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccns4)-c5ccccc5)CC)c1	5.7
56	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(OC)cc(OC)c4)-c5ccccc5)CC)c1	5.7
57	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc5CCCc5s4)-c6ccccc6)CC)c1	5.7
58	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(c(c4C)C)C)-c5ccccc5)CC)c1	5.7
59	Fc1cc(N)c(F)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.7
60	Oc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1N	5.7
61	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(s4)SC)-c5ccccc5)CC)c1	5.7
62	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5C[C@@H](Oc5c4)C)-c6ccccc6)CC)c1	5.7
63	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.7
64	Fc1cc(cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1)C	5.7

65	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4N)-c5ccccc5)CC)c1	5.7
66	Oc1ccc2c(OCO2)c1-c3c(c(n(n3)-c4ccccc4-c5cccc(OCC([O-])=O)c5)CC)-c6ccccc6	5.7
67	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cn5ccsc5c4)-c6ccccc6)CC)c1	5.7
68	Sc1ccc(F)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.7
69	OCc1c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)ccs1	5.7
70	Fc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1O	5.7
71	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4cc[nH]5)-c6ccccc6)CC)c1	5.6
72	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(-n4cc(cc4C)C)n3)-c5ccccc5)CC)c1	5.6
73	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(c5c4nsn5)C)-c6ccccc6)CC)c1	5.6
74	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cscc4C)-c5ccccc5)CC)c1	5.6
75	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4OC)-c5ccccc5)CC)c1	5.6
76	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(cc4)/C=C\C)-c5ccccc5)CC)c1	5.6
77	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(c4)cns5)-c6ccccc6)CC)c1	5.6
78	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4csc5ccccc54)-c6ccccc6)CC)c1	5.6
79	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(N4CCSCC4)n3)-c5ccccc5)CC)c1	5.6
80	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(N4CC[C@H]5C[C@H]54)n3)-c6ccccc6)CC)c1	5.6
81	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(N4CCOCC4)n3)-c5ccccc5)CC)c1	5.6
82	OCc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.6
83	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccs4)-c5ccccc5)CC)c1	5.6
84	Clc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1C	5.6
85	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4NCC5)-c6ccccc6)CC)c1	5.6
86	Fc1c(O)c(O)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.6
87	Oc1c(c(ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C)C	5.6
88	Oc1cc(cc(c1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C)C	5.6
89	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4[nH]cc5C)-c6ccccc6)CC)c1	5.6
90	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4c(N)ccs4)-c5ccccc5)CC)c1	5.6
91	Fc1ccc(O)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.6
92	Oc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1[N+]([O-])=O	5.6
93	FC(F)(F)c1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.6
94	Oc1c(O)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1O	5.6
95	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(NC)c4)-c5ccccc5)CC)c1	5.6
96	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5ccoc54)-c6ccccc6)CC)c1	5.6
97	Clc1c(F)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1	5.6
98	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccoc4C)-c5ccccc5)CC)c1	5.6
99	Oc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1COC	5.6
100	Oc1cc(CC)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.6
101	O[C@H](c1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1)C	5.6
102	Fc1c(SC)ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.6
103	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5COCCc5c4)-c6ccccc6)CC)c1	5.6
104	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4NC)-c5ccccc5)CC)c1	5.6
105	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4OCO5)-c6ccccc6)CC)c1	5.6
106	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5cc[nH]c54)-c6ccccc6)CC)c1	5.6
107	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(s4)CC)-c5ccccc5)CC)c1	5.6
108	Sc1c(N)ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.6

109	Fc1cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)ccc1C	5.6
110	Fc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c(N)c1	5.6
111	[O-][N+](=O)c1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1N	5.6
112	OCc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1	5.6
113	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(c4C)C)-c5ccccc5)CC)c1	5.6
114	Clc1cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c(N)cc1C	5.6
115	ONc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1	5.6
116	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(cc4)C=C)-c5ccccc5)CC)c1	5.6
117	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5ccccc54)-c6ccccc6)CC)c1	5.6
118	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(-n4cc(c5ccccc54)C)n3)-c6ccccc6)CC)c1	5.6
119	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc5c(s4)CCCC5)-c6ccccc6)CC)c1	5.5
120	Fc1cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc6cc[nH]c16	5.5
121	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(-n4ccc5ccccc54)n3)-c6ccccc6)CC)c1	5.5
122	Clc1ccc(F)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.5
123	Oc1c(N)cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.5
124	Clc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c(N)c1	5.5
125	Oc1c2ccoc2ccc1-c3c(c(n(n3)-c4ccccc4-c5cccc(OCC([O-])=O)c5)CC)-c6ccccc6	5.5
126	FC(F)c1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.5
127	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(CC)c4)-c5ccccc5)CC)c1	5.5
128	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(OCC#C)c4)-c5ccccc5)CC)c1	5.5
129	Fc1c(NC)c(F)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.5
130	Oc1c(O)cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.5
131	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4NN)-c5ccccc5)CC)c1	5.5
132	Fc1cc(F)c(F)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.5
133	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(SCC)c4)-c5ccccc5)CC)c1	5.5
134	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(N4CCCCC4)n3)-c5ccccc5)CC)c1	5.5
135	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(NN)c4)-c5ccccc5)CC)c1	5.5
136	Oc1c(N)ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.5
137	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(sc4C)C)-c5ccccc5)CC)c1	5.5
138	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(c(s4)C)C)-c5ccccc5)CC)c1	5.5
139	Oc1nc2ccc(-c3c(c(n(n3)-c4ccccc4-c5cccc(OCC([O-])=O)c5)CC)-c6ccccc6)cc2o1	5.5
140	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=Cc5ccccc5OC4)-c6ccccc6)CC)c1	5.5
141	Clc1c(O)c(O)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.5
142	Sc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1	5.5
143	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(C5CC5)cc4)-c6ccccc6)CC)c1	5.5
144	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(CC)cc4)-c5ccccc5)CC)c1	5.5
145	Oc1cc(N)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.5
146	Fc1ccc2c(c(-c3c(c(n(n3)-c4ccccc4-c5cccc(OCC([O-])=O)c5)CC)-c6ccccc6)cs2)c1	5.5
147	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4nco5)-c6ccccc6)CC)c1	5.5
148	Clc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1	5.5
149	Oc1cc(O)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.5
150	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(c4)C)-c5ccccc5)CC)c1	5.5
151	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(c4)CC=C)-c5ccccc5)CC)c1	5.5
152	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(cs4)C)-c5ccccc5)CC)c1	5.5

153	Oc1cccc(N)c1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.5
154	Oc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.5
155	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(c(s4)CC)C)-c5ccccc5)CC)c1	5.5
156	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(N4CCCC4)n3)-c5ccccc5)CC)c1	5.5
157	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccncc4N)-c5ccccc5)CC)c1	5.5
158	FC(F)c1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1	5.5
159	Clc1cc(Cl)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.5
160	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(cc4C)C)-c5ccccc5)CC)c1	5.5
161	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(NCC5)c4)-c6ccccc6)CC)c1	5.5
162	Oc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1C	5.5
163	Clc1ccc(s1)-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.5
164	OCc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1O	5.5
165	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(C(C)C)cc4)-c5ccccc5)CC)c1	5.5
166	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(cc4)C#CC)-c5ccccc5)CC)c1	5.5
167	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(CCC)c4)-c5ccccc5)CC)c1	5.5
168	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4csn5)-c6ccccc6)CC)c1	5.5
169	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4ocn5)-c6ccccc6)CC)c1	5.5
170	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)[C@@H](C4CC4)CC)-c5ccccc5)CC)c1	5.5
171	Clc1c(N)cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.5
172	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5ccsc54)-c6ccccc6)CC)c1	5.5
173	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(CCC)cc4)-c5ccccc5)CC)c1	5.5
174	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4cco5)-c6ccccc6)CC)c1	5.5
175	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4nc[nH]5)-c6ccccc6)CC)c1	5.5
176	Fc1c(ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1C)C	5.5
177	Fc1cc(ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C#C	5.5
178	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(SC)cc4)-c5ccccc5)CC)c1	5.5
179	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cocc4)-c5ccccc5)CC)c1	5.5
180	Fc1c(NC)ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.5
181	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccsc4N)-c5ccccc5)CC)c1	5.5
182	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(OCOC)c4)-c5ccccc5)CC)c1	5.5
183	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4CCN5)-c6ccccc6)CC)c1	5.5
184	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(c(OC)c4)C)-c5ccccc5)CC)c1	5.5
185	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5ccoc5c4)-c6ccccc6)CC)c1	5.5
186	Fc1c(cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	5.5
187	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccsc4C)-c5ccccc5)CC)c1	5.5
188	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(c4)cc(o5)C)-c6ccccc6)CC)c1	5.5
189	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(OC)c4N)-c5ccccc5)CC)c1	5.5
190	Clc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c(F)c1C	5.5
191	Oc1cc2c(OCC2)cc1-c3c(c(n(n3)-c4ccccc4-c5cccc(OCC([O-])=O)c5)CC)-c6ccccc6	5.5
192	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(C(C)C)c4)-c5ccccc5)CC)c1	5.5
193	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(c4)cc[nH]5)-c6ccccc6)CC)c1	5.5
194	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(s4)N)-c5ccccc5)CC)c1	5.5
195	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4c5c(OCO5)cs4)-c6ccccc6)CC)c1	5.5
196	FC(F)Oc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.5

197	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=CCCCCCC4)-c5ccccc5)CC)c1	5.5
198	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(c4)CSC)-c5ccccc5)CC)c1	5.5
199	Fc1c2cc[nH]c2ccc1-c3c(c(n(n3)-c4ccccc4-c5cccc(OCC([O-])=O)c5)CC)-c6ccccc6	5.5
200	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4occ5C)-c6ccccc6)CC)c1	5.5
201	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(C(C)=C)c4)-c5ccccc5)CC)c1	5.5
202	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(OC)cc4)-c5ccccc5)CC)c1	5.4
203	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(cc(OC)c4)C)-c5ccccc5)CC)c1	5.4
204	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=Cc5ccccc5C4)-c6ccccc6)CC)c1	5.4
205	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4OCC5)-c6ccccc6)CC)c1	5.4
206	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4ncs5)-c6ccccc6)CC)c1	5.4
207	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc5c(s4)cc[nH]5)-c6ccccc6)CC)c1	5.4
208	Clc1c(OC)cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.4
209	O=[S@@](c1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1)C	5.4
210	Fc1cccc(N)c1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.4
211	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cnsc4C)-c5ccccc5)CC)c1	5.4
212	Clc1cc(ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	5.4
213	Clc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c(F)c1	5.4
214	Clc1c(O)cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.4
215	Fc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.4
216	Fc1c(N)cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.4
217	Clc1c(Cl)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1	5.4
218	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(c4)C#C)-c5ccccc5)CC)c1	5.4
219	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(c4)C=C)-c5ccccc5)CC)c1	5.4
220	Clc1cc(O)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.4
221	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc[nH]c4C)-c5ccccc5)CC)c1	5.4
222	Oc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1N	5.4
223	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cnc(s4)C)-c5ccccc5)CC)c1	5.4
224	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5ccccc5c4)-c6ccccc6)CC)c1	5.4
225	Clc1c(O)c(O)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.4
226	Clc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1O	5.4
227	Clc1c(O)ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.4
228	Clc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1F	5.4
229	Fc1cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c(F)cc1C	5.4
230	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4C=C)-c5ccccc5)CC)c1	5.4
231	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4COCO5)-c6ccccc6)CC)c1	5.4
232	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4csc(CCC)c4)-c5ccccc5)CC)c1	5.4
233	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(nco5)c4)-c6ccccc6)CC)c1	5.4
234	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(s4)OC)-c5ccccc5)CC)c1	5.4
235	Oc1c(O)c(O)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.4
236	Clc1cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)co1	5.4
237	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4csc(CC)c4)-c5ccccc5)CC)c1	5.4
238	Oc1c(O)c(OC)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.4
239	Oc1ccc([N+]([O-])=O)c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.4
240	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5CCCc5c4)-c6ccccc6)CC)c1	5.4

241	Oc1cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)ccc1C	5.4
242	Oc1c(O)ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.4
243	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(sc4)C)-c5ccccc5)CC)c1	5.4
244	Clc1cccc(O)c1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.4
245	Fc1cc(ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	5.4
246	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(sc4C)N)-c5ccccc5)CC)c1	5.4
247	Sc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.4
248	Oc1cc(cc(O)c1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	5.4
249	Fc1ccncc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.4
250	Oc1cc(ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	5.4
251	Fc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1C	5.4
252	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(c4)COC)-c5ccccc5)CC)c1	5.4
253	SCc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1	5.4
254	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)/C=C/C(C)=C)-c4ccccc4)CC)c1	5.4
255	Sc1ccccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.4
256	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(CCS5)c4)-c6ccccc6)CC)c1	5.4
257	Fc1cc(NC)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.4
258	Clc1c(O)c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)ccc1C	5.4
259	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(c4)ccs5)-c6ccccc6)CC)c1	5.4
260	FCCc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1	5.4
261	Clc1ccsc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.4
262	FC(F)(c1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1)C	5.4
263	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(CCO5)c4)-c6ccccc6)CC)c1	5.4
264	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=CSCCO4)-c5ccccc5)CC)c1	5.4
265	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(OC)c(N)c4)-c5ccccc5)CC)c1	5.4
266	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=COCCC4)-c5ccccc5)CC)c1	5.4
267	Oc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1CC	5.4
268	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4csc5CCCCc54)-c6ccccc6)CC)c1	5.4
269	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4cc(o5)C)-c6ccccc6)CC)c1	5.4
270	Fc1ccc(s1)-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.4
271	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(cc4)CC=C)-c5ccccc5)CC)c1	5.4
272	FC(c1c(c(n(n1)-c2ccccc2-c3cccc(OCC([O-])=O)c3)CC)-c4ccccc4)=C(C)C	5.4
273	Oc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1C	5.4
274	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc5ccsc5s4)-c6ccccc6)CC)c1	5.4
275	Fc1cc(N)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.3
276	Fc1ccccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.3
277	Clc1c(F)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c(F)c1	5.3
278	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(c4)cco5)-c6ccccc6)CC)c1	5.3
279	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(CC)c(s4)C)-c5ccccc5)CC)c1	5.3
280	Clc1c(cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	5.3
281	Fc1c(OC)c(F)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.3
282	Clc1cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cs1	5.3
283	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(-n4cccc4CC)n3)-c5ccccc5)CC)c1	5.3
284	Oc1cc(O)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.3

285	Fc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1	5.3
286	Clc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c(c1)C	5.3
287	Clc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1C	5.3
288	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4c(cc[nH]4)C)-c5ccccc5)CC)c1	5.3
289	OCc1ccc(s1)-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.3
290	Oc1cc(cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1)C	5.3
291	Clc1csc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.3
292	Clc1ccc(F)c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.3
293	Clc1ccc(O)c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.3
294	Clc1cc(F)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.3
295	Fc1c(O)ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.3
296	Oc1c(OC)cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.3
297	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=CCCCCC4)-c5ccccc5)CC)c1	5.3
298	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(cc(c4)C)C)-c5ccccc5)CC)c1	5.3
299	Clc1c(F)cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.3
300	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(C(C)C)cs4)-c5ccccc5)CC)c1	5.3
301	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc[nH+]c(N)c4)-c5ccccc5)CC)c1	5.3
302	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cscc4N)-c5ccccc5)CC)c1	5.3
303	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(ncs5)c4)-c6ccccc6)CC)c1	5.3
304	O=[S@](c1ccccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	5.3
305	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4CC=C)-c5ccccc5)CC)c1	5.3
306	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C=C(C)C)-c4ccccc4)CC)c1	5.3
307	Oc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1	5.3
308	Oc1c(cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)CO	5.3
309	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc([C@@H]5CO5)cc4)-c6ccccc6)CC)c1	5.3
310	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(OCC)c4)-c5ccccc5)CC)c1	5.3
311	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cscc4)-c5ccccc5)CC)c1	5.3
312	ClC=1CCCCC1c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.3
313	Clc1ccccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.3
314	Clc1c(F)ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.3
315	Oc1cccc(O)c1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.3
316	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(N#C)cc4)-c5ccccc5)CC)c1	5.3
317	Fc1cc(F)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.3
318	Clc1ccc(N)c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.3
319	O=[S@@](c1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1)C	5.3
320	Fc1cc(OC)c(F)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.3
321	Fc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1CO	5.3
322	OCc1c(O)ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.3
323	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4n[nH]n5)-c6ccccc6)CC)c1	5.3
324	Clc1ccc(Cl)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.3
325	Fc1c(OC)cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.3
326	Fc1cc(F)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1O	5.3
327	Oc1c(OC)ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.3
328	Fc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1N	5.2

329	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(OCC=C)c4)-c5ccccc5)CC)c1	5.2
330	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(s4)C)-c5ccccc5)CC)c1	5.2
331	Fc1ccc(F)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.2
332	Fc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1O	5.2
333	[O-][N+](=O)c1ccccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.2
334	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5cnsc5c4)-c6ccccc6)CC)c1	5.2
335	Clc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c(OC)c1	5.2
336	Oc1c(cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	5.2
337	Fc1cc(OC)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.2
338	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc[nH+]c4N)-c5ccccc5)CC)c1	5.2
339	Fc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1F	5.2
340	Fc1c(O)c(O)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.2
341	Fc1cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)ccc1CC	5.2
342	Oc1nc2ccc(-c3c(c(n(n3)-c4ccccc4-c5cccc(OCC([O-])=O)c5)CC)-c6ccccc6)cc2s1	5.2
343	Fc1c(F)c(O)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.2
344	Fc1c(OC)c(F)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.2
345	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccncc4)-c5ccccc5)CC)c1	5.2
346	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=CC[C@@H](CC4)C)-c5ccccc5)CC)c1	5.2
347	Clc1c(N)ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.2
348	Oc1cc(c(cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C)C	5.2
349	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4c[nH+]c(N)cc4)-c5ccccc5)CC)c1	5.2
350	Fc1c(F)c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)ccc1C	5.2
351	Fc1cnccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.2
352	Oc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c([N+]([O-])=O)c1	5.2
353	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4c(c(c[nH]4)C)C)-c5ccccc5)CC)c1	5.2
354	Fc1c(N)ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.2
355	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4CCO5)-c6ccccc6)CC)c1	5.2
356	Clc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1N	5.2
357	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=CCCCO4)-c5ccccc5)CC)c1	5.2
358	Fc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1N	5.2
359	I/C=C/c1c(c(n(n1)-c2ccccc2-c3cccc(OCC([O-])=O)c3)CC)-c4ccccc4	5.2
360	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(nsc5c4)C)-c6ccccc6)CC)c1	5.2
361	Fc1ccc(cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	5.2
362	Oc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1OC	5.2
363	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)CCCC=C)-c4ccccc4)CC)c1	5.2
364	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(SC)c(c4)C)-c5ccccc5)CC)c1	5.2
365	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=CCOCC4)-c5ccccc5)CC)c1	5.2
366	Fc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c(O)c1	5.2
367	Clc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c(O)c1	5.2
368	Fc1c(F)cc(F)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.2
369	[O-][N+](OCc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1)=O	5.2
370	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccnc(c4)C)-c5ccccc5)CC)c1	5.2
371	[O-][N+](=O)c1c(cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	5.2
372	Fc1c(OC)ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.2

373	ONc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.2
374	Fc1cccc(F)c1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.2
375	Clc1cc(F)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.2
376	Clc1cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)ccc1C	5.2
377	Clc1ccc(c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1)C	5.2
378	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(OCO5)c4)-c6ccccc6)CC)c1	5.2
379	FC(F)(F)c1ccc(s1)-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.2
380	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=CCCC4)-c5ccccc5)CC)c1	5.2
381	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(cc4)C#C)-c5ccccc5)CC)c1	5.2
382	OCCc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.2
383	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(s4)C(C)C)-c5ccccc5)CC)c1	5.2
384	Fc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1OCC	5.2
385	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)[C@@]4(CO4)C)-c5ccccc5)CC)c1	5.2
386	Fc1cc(O)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.2
387	Fc1ccc(OC)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.2
388	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4c(cns4)C)-c5ccccc5)CC)c1	5.2
389	Fc1c(N)c(F)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.2
390	Oc1cccc(OC)c1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.2
391	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=CCC=CC4)-c5ccccc5)CC)c1	5.2
392	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(CCC)c(s4)C)-c5ccccc5)CC)c1	5.2
393	Fc1cc(F)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.2
394	Clc1c(cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1C)C	5.2
395	Fc1ccc(NC)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.1
396	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(OC)n4)-c5ccccc5)CC)c1	5.1
397	Clc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.1
398	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)[C@H](OC)CC)-c4ccccc4)CC)c1	5.1
399	Fc1cccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1C	5.1
400	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(N(C4CC4)CC)n3)-c5ccccc5)CC)c1	5.1
401	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(OC)c(c4)C)-c5ccccc5)CC)c1	5.1
402	Fc1c(F)cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.1
403	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccco4)-c5ccccc5)CC)c1	5.1
404	FCCCc1c(c(n(n1)-c2ccccc2-c3cccc(OCC([O-])=O)c3)CC)-c4ccccc4	5.1
405	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(c4)/C=C/C)-c5ccccc5)CC)c1	5.1
406	Clc1c(Cl)cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.1
407	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(c4)CC#N)-c5ccccc5)CC)c1	5.1
408	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cnc(OC)cc4)-c5ccccc5)CC)c1	5.1
409	Fc1c(F)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1O	5.1
410	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4csc(c4C)C)-c5ccccc5)CC)c1	5.1
411	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=CC=CCC4)-c5ccccc5)CC)c1	5.1
412	Fc1cc(F)c(N)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.1
413	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C=4C=COCC4)-c5ccccc5)CC)c1	5.1
414	Fc1c(O)c(OC)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.1
415	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4c[nH+]c(N)c(c4)C)-c5ccccc5)CC)c1	5.1
416	Oc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c(c1C)C	5.1

417	Oc1c(O)cc(cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	5.1
418	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(ccc4N)C)-c5ccccc5)CC)c1	5.1
419	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(scn5)c4)-c6ccccc6)CC)c1	5.1
420	Clc1ccc(OC)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.1
421	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=CCCCC4)-c5ccccc5)CC)c1	5.1
422	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(c4OC)C)-c5ccccc5)CC)c1	5.1
423	Fc1c(O)cccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.1
424	Oc1cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c(O)cc1C	5.1
425	O[C@@H](/C=C/c1c(c(n(n1)-c2ccccc2-c3cccc(OCC([O-])=O)c3)CC)-c4ccccc4)C	5.1
426	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)/C(CC)=C/C)-c4ccccc4)CC)c1	5.1
427	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C(CC)=C)-c4ccccc4)CC)c1	5.1
428	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C(CCC)=C)-c4ccccc4)CC)c1	5.1
429	Oc1cc(O)c(O)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.0
430	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc(N)c(C[N+])c4)-c5ccccc5)CC)c1	5.0
431	Clc1ccc(o1)-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.0
432	Fc1c(cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1C)C	5.0
433	Fc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c(c1)C	5.0
434	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4nccs4)-c5ccccc5)CC)c1	5.0
435	Clc1cc(cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1)C	5.0
436	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)CCC=C)-c4ccccc4)CC)c1	5.0
437	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc(c4)C#N)-c5ccccc5)CC)c1	5.0
438	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5c4nn[nH]5)-c6ccccc6)CC)c1	5.0
439	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(cc(c4N)C)C)-c5ccccc5)CC)c1	5.0
440	Clc1cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc6c1cc[nH]6	5.0
441	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(-[n+]4ccccc4N)n3)-c5ccccc5)CC)c1	5.0
442	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)[C@H](OC)C)-c4ccccc4)CC)c1	5.0
443	Oc1cc(OC)ccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.0
444	Clc1nc2ccc(-c3c(c(n(n3)-c4ccccc4-c5cccc(OCC([O-])=O)c5)CC)-c6ccccc6)cc2o1	5.0
445	Clc1cc(Cl)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.0
446	Clc1cc(F)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1O	5.0
447	Clc1c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)ccs1	5.0
448	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5cnoc54)-c6ccccc6)CC)c1	5.0
449	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cccc5cn[nH]c54)-c6ccccc6)CC)c1	5.0
450	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(-n4cccc4)n3)-c5ccccc5)CC)c1	5.0
451	Clc1c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc(s1)C	5.0
452	S=C1C=C(SS1)c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	5.0
453	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5COCc5c4)-c6ccccc6)CC)c1	5.0
454	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(ccc4C)C)-c5ccccc5)CC)c1	5.0
455	Clc1c(OC)ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	5.0
456	Fc1cccc(c1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	5.0
457	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=CC=CC4)-c5ccccc5)CC)c1	5.0
458	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cnccc4)-c5ccccc5)CC)c1	5.0
459	OC/C=C(/c1c(c(n(n1)-c2ccccc2-c3cccc(OCC([O-])=O)c3)CC)-c4ccccc4)C	5.0
460	Clc1cncc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	4.9

461	[O-][n+]1ccccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	4.9
462	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=C(OCCC4)C)-c5ccccc5)CC)c1	4.9
463	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(N4CSCC4)n3)-c5ccccc5)CC)c1	4.9
464	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C(C)=C)-c4ccccc4)CC)c1	4.9
465	Oc1c(OC)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1N	4.9
466	Fc1c(F)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1OC	4.9
467	Clc1cccn1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	4.9
468	Fc1ccc(c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1)C	4.9
469	Fc1cc(F)c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1C	4.9
470	Fc1cc(O)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	4.9
471	Clc1cccc(c1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	4.9
472	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(c[nH+]c4N)C)-c5ccccc5)CC)c1	4.9
473	Oc1nc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cs1	4.9
474	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=CCC=C4)-c5ccccc5)CC)c1	4.9
475	S=C1C(c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)=CSS1	4.9
476	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=CCCOC4)-c5ccccc5)CC)c1	4.9
477	Fc1cc(F)cc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1N	4.9
478	Fc1cccc(O)c1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	4.8
479	OCc1ccccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	4.8
480	ClC(c1c(c(n(n1)-c2ccccc2-c3cccc(OCC([O-])=O)c3)CC)-c4ccccc4)=C	4.8
481	Fc1ccc(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1SC	4.8
482	Clc1ccc(cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	4.8
483	OC/C(c1c(c(n(n1)-c2ccccc2-c3cccc(OCC([O-])=O)c3)CC)-c4ccccc4)=C\C	4.8
484	SCC1(CC1)c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	4.8
485	Clc1cccc(N)c1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	4.8
486	Oc1ccccc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	4.7
487	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccc5c(c(co5)C)c4)-c6ccccc6)CC)c1	4.7
488	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(-[n+]4ccccc4)n3)-c5ccccc5)CC)c1	4.7
489	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4C#C)-c5ccccc5)CC)c1	4.7
490	Fc1cc(F)cc(O)c1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	4.7
491	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4cc(c(cc4N)C)C)-c5ccccc5)CC)c1	4.7
492	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)C4=COCC4)-c5ccccc5)CC)c1	4.7
493	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(-[n+]4cccc(N)c4)n3)-c5ccccc5)CC)c1	4.6
494	BrC(c1c(c(n(n1)-c2ccccc2-c3cccc(OCC([O-])=O)c3)CC)-c4ccccc4)=C	4.6
495	Oc1ccc(CC)cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5	4.6
496	Clc1cc(O)c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)cc1C	4.6
497	Fc1ccc(O)c(-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)c1	4.5
498	Oc1cccc(c1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	4.5
499	Oc1ccc(cc1-c2c(c(n(n2)-c3ccccc3-c4cccc(OCC([O-])=O)c4)CC)-c5ccccc5)C	4.5
500	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4CC)-c5ccccc5)CC)c1	4.5

Table 5

SMILE and predicted pIC_{50} values for Series 2 derivatives.

N°	SMILES	$_{Pred}pIC_{50}$
1	Oc1c(OC)cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	6.0
2	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5c[nH]cc5)CC)c1	5.9
3	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc[nH]5)CC)c1	5.9
4	Oc1c(N)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.9
5	Oc1c(sc(n1)N)-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.9
6	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(c(NC)c5)C)CC)c1	5.8
7	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc(NCC)c4)c(n3)-c5ccccc5)CC)c1	5.8
8	Fc1cccc(O)c1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.8
9	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cnc5c(c4)cc[nH]5)c(n3)-c6ccccc6)CC)c1	5.8
10	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5coc(N)c5)CC)c1	5.8
11	Clc1c(N)cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.8
12	Oc1cc(O)c(O)cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.8
13	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(s5)N)CC)c1	5.8
14	Sc1c(N)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.8
15	Oc1c(O)cc(cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.7
16	Oc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1OC	5.7
17	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5c(c4)cc[nH]5)c(n3)-c6ccccc6)CC)c1	5.7
18	FC(F)c1ccccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.7
19	Oc1cc(ncc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.7
20	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5NN)CC)c1	5.7
21	Brc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)co1	5.7
22	Brc1ccc([nH]1)-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.7
23	Oc1c(O)cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.7
24	Clc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1O	5.7
25	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5c(OC)ccs5)CC)c1	5.7
26	Clc1c(N)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.7
27	Fc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc6cc[nH]c16	5.7
28	Oc1ccncc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.7
29	Oc1ccc([N+]([O-])=O)c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.7
30	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5CCNc54)c(n3)-c6ccccc6)CC)c1	5.7
31	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(N)cc5)CC)c1	5.7
32	Fc1c(N)cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.7
33	Oc1cc(O)ccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.7
34	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccc(NC)c5)CC)c1	5.7
35	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(NN)cc5)CC)c1	5.7
36	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5c4nn[nH]5)c(n3)-c6ccccc6)CC)c1	5.7
37	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5C#C)CC)c1	5.7
38	Clc1cccn1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.7
39	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc(N)c[nH]5)CC)c1	5.7
40	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cncc(c4)C)c(n3)-c5ccccc5)CC)c1	5.7
41	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5c6c(OCO6)cs5)CC)c1	5.7
42	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc(N)c(c4)C)c(n3)-c5ccccc5)CC)c1	5.7
43	Oc1ccc(O)cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.7

44	Clc1c(N)cc(O)c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.7
45	Oc1c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cccn1	5.7
46	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc6c(n[nH]n6)c5)CC)c1	5.7
47	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc(c4)/C=C/C)c(n3)-c5ccccc5)CC)c1	5.6
48	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc(N)c(s5)C)CC)c1	5.6
49	Fc1ccc(NC)cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.6
50	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cnsc5C)CC)c1	5.6
51	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5ccoc54)c(n3)-c6ccccc6)CC)c1	5.6
52	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(C4=CCCCC4)c(n3)-c5ccccc5)CC)c1	5.6
53	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cocc5)CC)c1	5.6
54	Oc1cc2c(OCC2)cc1-c3c(nn(c3CC)-c4ccccc4-c5cccc(OCC([O-])=O)c5)-c6ccccc6	5.6
55	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5c4cc[nH]5)c(n3)-c6ccccc6)CC)c1	5.6
56	Fc1c(O)c(O)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.6
57	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc(C(C)C)c4)c(n3)-c5ccccc5)CC)c1	5.6
58	Fc1cc(N)ccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.6
59	Oc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cn1	5.6
60	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5/C=C/C)CC)c1	5.6
61	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5c4OCC5)c(n3)-c6ccccc6)CC)c1	5.6
62	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc6c([nH]5)ncs6)CC)c1	5.6
63	Oc1c(N)cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.6
64	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(s5)C)CC)c1	5.6
65	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-n4cccc4)c(n3)-c5ccccc5)CC)c1	5.6
66	Clc1cncc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.6
67	Sc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.6
68	Oc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)ccn1	5.6
69	Clc1c(O)c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)ccc1C	5.6
70	Fc1c(NC)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.6
71	Fc1ccc(F)cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.6
72	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc6c(OCCO6)c5)CC)c1	5.6
73	Oc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1CC	5.6
74	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5NCC)CC)c1	5.6
75	Clc1ccc(O)c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.6
76	Oc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1OC	5.6
77	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5c(cc(s5)N)C)CC)c1	5.6
78	Oc1ccoc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.6
79	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccc(C(C)=C)c5)CC)c1	5.6
80	Fc1cc(N)c(F)cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.6
81	Fc1cc(O)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.6
82	Fc1c(N)c(F)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.6
83	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc(sc5C)N)CC)c1	5.6
84	Fc1cncc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.6
85	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(CCC)cc5)CC)c1	5.6
86	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)C=5C=CCC5)CC)c1	5.6
87	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4c(CC)ccs4)c(n3)-c5ccccc5)CC)c1	5.6

88	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccc(N)c5C#N)CC)c1	5.6
89	Fc1ccncc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.6
90	Oc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)ccc1C	5.6
91	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5c4n[nH]n5)c(n3)-c6ccccc6)CC)c1	5.6
92	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(cc5OC)C)CC)c1	5.6
93	Clc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)co1	5.6
94	Oc1ccc(CC)cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.6
95	Oc1c(cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.6
96	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.6
97	Clc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.6
98	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(s5)NC)CC)c1	5.5
99	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(sc4C)C)c(n3)-c5ccccc5)CC)c1	5.5
100	Clc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1C	5.5
101	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc(c(c4)C)C)c(n3)-c5ccccc5)CC)c1	5.5
102	Fc1ccc(cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.5
103	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(ccc4C)C)c(n3)-c5ccccc5)CC)c1	5.5
104	Clc1ncc(s1)-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.5
105	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(c[nH]4)C)c(n3)-c5ccccc5)CC)c1	5.5
106	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cnccc5)CC)c1	5.5
107	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc6cc[nH]c6s5)CC)c1	5.5
108	FC(F)Oc1ccccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.5
109	Clc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1O	5.5
110	Clc1cccc(F)c1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.5
111	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(cc5)CC=C)CC)c1	5.5
112	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccns5)CC)c1	5.5
113	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(cc5)C#CC)CC)c1	5.5
114	FC(F)Oc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.5
115	Clc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.5
116	Oc1c(OC)cc(cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.5
117	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc([C@H]6CO6)cc5)CC)c1	5.5
118	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccccc4C5CC5)c(n3)-c6ccccc6)CC)c1	5.5
119	Clc1cc(cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1)C	5.5
120	FC(F)(F)c1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.5
121	Oc1c(c(ccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C)C	5.5
122	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cn(c(c4)C)C)c(n3)-c5ccccc5)CC)c1	5.5
123	Clc1csc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.5
124	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc([nH]c4)C)c(n3)-c5ccccc5)CC)c1	5.5
125	Oc1ccc(c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1)C	5.5
126	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccs5)CC)c1	5.5
127	Clc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)ccc1C	5.5
128	OCc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cs1	5.5
129	Fc1c(N)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.5
130	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccc(N(C)C)c5)CC)c1	5.5
131	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(N)c(OC)c5)CC)c1	5.5

132	Clc1ccccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.5
133	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5N(C)C)CC)c1	5.5
134	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(C(C)=C)cc5)CC)c1	5.5
135	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5c(SC)ccs5)CC)c1	5.5
136	Oc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)ccc1CC	5.5
137	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc(NC)c(c4)C)c(n3)-c5ccccc5)CC)c1	5.5
138	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc(c(CC)c4)C)c(n3)-c5ccccc5)CC)c1	5.5
139	Oc1c2c(ccc1-c3c(nn(c3CC)-c4ccccc4-c5cccc(OCC([O-])=O)c5)-c6ccccc6)cccn2	5.5
140	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(CC)cc5)CC)c1	5.5
141	Fc1cc(ccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.5
142	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccc6c5nco6)CC)c1	5.5
143	Oc1c(cc(cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C)C	5.5
144	Fc1ccc(O)c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.5
145	Fc1ccccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.5
146	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc(c4N)C)c(n3)-c5ccccc5)CC)c1	5.5
147	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc6c(c(co6)C)c5)CC)c1	5.5
148	FC(F)Oc1ccsc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.5
149	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cnc(OC)cc5)CC)c1	5.5
150	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc(N)c(N)c4)c(n3)-c5ccccc5)CC)c1	5.5
151	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(N)c(s4)CC)c(n3)-c5ccccc5)CC)c1	5.5
152	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(C4=CC=CC4)c(n3)-c5ccccc5)CC)c1	5.5
153	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccccc4SC)c(n3)-c5ccccc5)CC)c1	5.5
154	Fc1cccc(c1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.5
155	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cn5CCCc5c4)c(n3)-c6ccccc6)CC)c1	5.5
156	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5c[nH]cc5C)CC)c1	5.5
157	FCCc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.5
158	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5csnc5)CC)c1	5.5
159	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(c(cc4N)C)C)c(n3)-c5ccccc5)CC)c1	5.5
160	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc(C(C)C)cc4)c(n3)-c5ccccc5)CC)c1	5.5
161	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5CCCc5c4)c(n3)-c6ccccc6)CC)c1	5.5
162	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc6ccoc6c5)CC)c1	5.5
163	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc6c(s5)ccs6)CC)c1	5.5
164	Clc1cc(O)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.5
165	OCc1csc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.5
166	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5NC)CC)c1	5.5
167	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(N#C)cc5)CC)c1	5.5
168	Clc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c(F)c1	5.5
169	Fc1cc(ccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C#C	5.5
170	Oc1cccc(O)c1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.5
171	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cn(cc4)C)c(n3)-c5ccccc5)CC)c1	5.5
172	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc(C5CC5)cc4)c(n3)-c6ccccc6)CC)c1	5.5
173	Fc1c(cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.5
174	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cn5c(OCCC5)c4)c(n3)-c6ccccc6)CC)c1	5.5
175	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(cc5)/C=C\C)CC)c1	5.5

176	Oc1cccc(c1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.5
177	FC(F)Oc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.5
178	Clc1cc(ccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.5
179	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc6c(s5)cc[nH]6)CC)c1	5.5
180	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cncc(c5)C#C)CC)c1	5.5
181	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(s5)N(C)C)CC)c1	5.5
182	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc(N(C)C)cc4)c(n3)-c5ccccc5)CC)c1	5.5
183	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccc(OCC)c5)CC)c1	5.5
184	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc(OC)cs5)CC)c1	5.5
185	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc6c(nco6)c5)CC)c1	5.5
186	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc(SC)c(c4)C)c(n3)-c5ccccc5)CC)c1	5.5
187	Clc1c(O)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.5
188	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc(c4C)C)c(n3)-c5ccccc5)CC)c1	5.5
189	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5csc(N)c5)CC)c1	5.5
190	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5c(CCN5)c4)c(n3)-c6ccccc6)CC)c1	5.5
191	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc6ccccc6c5)CC)c1	5.5
192	Clc1cc(c(O)c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1)C	5.5
193	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc6c(OCO6)c5)CC)c1	5.5
194	FC(c1c(nn(c1CC)-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)=C(C)C	5.5
195	Clc1ccncc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.5
196	Fc1c(OCC)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.4
197	Clc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c(N)c1	5.4
198	Oc1cc(cc(c1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C)C	5.4
199	Fc1ccc(c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1)C	5.4
200	Clc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c(N)cc1C	5.4
201	Oc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1C	5.4
202	Oc1c(CC)cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.4
203	Clc1c(F)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.4
204	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(cc(c4N)C)C)c(n3)-c5ccccc5)CC)c1	5.4
205	Clc1c(cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.4
206	Fc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1O	5.4
207	Fc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1O	5.4
208	Sc1cccc(n1)-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.4
209	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(OC)cc5)CC)c1	5.4
210	Clc1c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)ccs1	5.4
211	Fc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cn1	5.4
212	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5c(CCCC5)c4)c(n3)-c6ccccc6)CC)c1	5.4
213	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(sc4N)C)c(n3)-c5ccccc5)CC)c1	5.4
214	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(OCC#C)cc5)CC)c1	5.4
215	Oc1c(cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1C)C	5.4
216	Oc1c(cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)CO	5.4
217	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5COCc5c4)c(n3)-c6ccccc6)CC)c1	5.4
218	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccc(OCC#C)c5)CC)c1	5.4
219	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4csc(C(C)C)c4)c(n3)-c5ccccc5)CC)c1	5.4

220	Oc1ccc(cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.4
221	Clc1ccc(s1)-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.4
222	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(c(s4)C)C)c(n3)-c5ccccc5)CC)c1	5.4
223	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccc(c5)C=C)CC)c1	5.4
224	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5c(cc(s5)C)C)CC)c1	5.4
225	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5c(c4)cc(o5)C)c(n3)-c6ccccc6)CC)c1	5.4
226	Oc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.4
227	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc6c(SCC6)c5)CC)c1	5.4
228	Clc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1C	5.4
229	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5c4OCCO5)c(n3)-c6ccccc6)CC)c1	5.4
230	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc(cs5)C)CC)c1	5.4
231	Sc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.4
232	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5c(ccs5)C)CC)c1	5.4
233	OCc1c(cc(s1)-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.4
234	Fc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1C	5.4
235	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc(c(c4C)C)C)c(n3)-c5ccccc5)CC)c1	5.4
236	Oc1c2cc[nH]c2ccc1-c3c(nn(c3CC)-c4ccccc4-c5cccc(OCC([O-])=O)c5)-c6ccccc6	5.4
237	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc(N)c4)c(n3)-c5ccccc5)CC)c1	5.4
238	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5N)CC)c1	5.4
239	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(C4=CCC=CC4)c(n3)-c5ccccc5)CC)c1	5.4
240	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc(c4)C)c(n3)-c5ccccc5)CC)c1	5.4
241	Clc1ccc(F)cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.4
242	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(c(c(c4)C)C)C)c(n3)-c5ccccc5)CC)c1	5.4
243	Oc1ccccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.4
244	Clc1ccsc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.4
245	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc6c(OCC6)c5)CC)c1	5.4
246	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(NC)cc5)CC)c1	5.4
247	Clc1cccc(c1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.4
248	Fc1cc(F)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.4
249	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(cc(N)c4)C)c(n3)-c5ccccc5)CC)c1	5.4
250	Clc1c(F)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.4
251	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(s5)CC)CC)c1	5.4
252	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccc(OC)c5)CC)c1	5.4
253	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(cc5)C)CC)c1	5.4
254	Fc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)ccc1C	5.4
255	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cocc5C)CC)c1	5.4
256	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(SC)o5)CC)c1	5.4
257	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc(C(C)C)cs5)CC)c1	5.4
258	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccccc4OCC)c(n3)-c5ccccc5)CC)c1	5.4
259	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5C)CC)c1	5.4
260	Clc1c(O)cc(O)c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.4
261	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5CCCc45)c(n3)-c6ccccc6)CC)c1	5.4
262	Clc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c(cc1C)C	5.4
263	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc6ccsc6s5)CC)c1	5.4

264	Fc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.4
265	Oc1nc2ccc(-c3c(nn(c3CC)-c4ccccc4-c5cccc(OCC([O-])=O)c5)-c6ccccc6)cc2s1	5.4
266	Clc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c(O)cc1C	5.4
267	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(c(OC)c5)C)CC)c1	5.4
268	Clc1cccc(O)c1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.4
269	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc5CCCc5s4)c(n3)-c6ccccc6)CC)c1	5.4
270	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc(N)cs5)CC)c1	5.4
271	Oc1c(OCC)cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.4
272	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(C4=COCC4)c(n3)-c5ccccc5)CC)c1	5.4
273	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc(CC)c4)c(n3)-c5ccccc5)CC)c1	5.4
274	Oc1c(OC)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.4
275	S=C(SC)c1c(nn(c1CC)-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4	5.4
276	Clc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1F	5.4
277	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5c(c4)cco5)c(n3)-c6ccccc6)CC)c1	5.4
278	Oc1cc(CC)ccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.4
279	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5c(N(CC5)C)c4)c(n3)-c6ccccc6)CC)c1	5.4
280	Clc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c(O)c1	5.4
281	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(NCC)cc5)CC)c1	5.4
282	Clc1ccc(F)c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.4
283	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc(oc5)C)CC)c1	5.4
284	Clc1c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc(s1)C	5.4
285	Oc1ccc(N)cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.4
286	Oc1c(CC=C)cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.4
287	Fc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c(c1)C	5.4
288	Oc1cc2c(OCO2)cc1-c3c(nn(c3CC)-c4ccccc4-c5cccc(OCC([O-])=O)c5)-c6ccccc6	5.4
289	Oc1cccc(n1)-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.4
290	[O-][N+](=O)c1c(N)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.4
291	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(cc(OC)c4)C)c(n3)-c5ccccc5)CC)c1	5.4
292	Clc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1N	5.4
293	Fc1c(O)cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.4
294	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc5c(s4)SCC5)c(n3)-c6ccccc6)CC)c1	5.3
295	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5c(cc[nH]5)C)CC)c1	5.3
296	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc(C5CC5)c4)c(n3)-c6ccccc6)CC)c1	5.3
297	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cscc5C)CC)c1	5.3
298	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5c(c[nH]c54)C)c(n3)-c6ccccc6)CC)c1	5.3
299	Clc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cs1	5.3
300	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc6ccoc6s5)CC)c1	5.3
301	Clc1c(Cl)cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.3
302	Clc1ccc(N)c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.3
303	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5cn[nH]c54)c(n3)-c6ccccc6)CC)c1	5.3
304	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc6c(scn6)c5)CC)c1	5.3
305	Oc1cc(ccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.3
306	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(s5)SC)CC)c1	5.3
307	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(s5)C(C)C)CC)c1	5.3

308	Oc1nc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cs1	5.3
309	Oc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1N	5.3
310	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc(sc5)C)CC)c1	5.3
311	FC(F)(c1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1)C	5.3
312	Clc1c(F)cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.3
313	Oc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.3
314	Fc1c(NC)c(F)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.3
315	Fc1c(cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1C)C	5.3
316	Clc1ccc(c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1)C	5.3
317	Clc1cccc(N)c1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.3
318	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc(N)c4N)c(n3)-c5ccccc5)CC)c1	5.3
319	FC(F)c1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.3
320	Oc1c(O)c(OC)ccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.3
321	Oc1cc2CCCc2cc1-c3c(nn(c3CC)-c4ccccc4-c5cccc(OCC([O-])=O)c5)-c6ccccc6	5.3
322	Clc1cc(Cl)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.3
323	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(CCC=C)c(n3)-c4ccccc4)CC)c1	5.3
324	Clc1c(O)c(O)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.3
325	OCc1c(O)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.3
326	[O-][N+](OCc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1)=O	5.3
327	Fc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c(OC)c1	5.3
328	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5c(NCC5)c4)c(n3)-c6ccccc6)CC)c1	5.3
329	O=C(N)c1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cs1	5.3
330	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccsc5C)CC)c1	5.3
331	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc(CCC)c4)c(n3)-c5ccccc5)CC)c1	5.3
332	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc6c(ocn6)c5)CC)c1	5.3
333	Oc1ccc2c(OCO2)c1-c3c(nn(c3CC)-c4ccccc4-c5cccc(OCC([O-])=O)c5)-c6ccccc6	5.3
334	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccc(c5)C#C)CC)c1	5.3
335	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5COCc54)c(n3)-c6ccccc6)CC)c1	5.3
336	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(c(s4)CC)C)c(n3)-c5ccccc5)CC)c1	5.3
337	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccoc5N)CC)c1	5.3
338	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5c4cc(o5)C)c(n3)-c6ccccc6)CC)c1	5.3
339	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc6ccsc6c5)CC)c1	5.3
340	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc6ccccc6s5)CC)c1	5.3
341	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc(CC)cs5)CC)c1	5.3
342	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(CC)c(s4)C)c(n3)-c5ccccc5)CC)c1	5.3
343	Clc1cc(F)ccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.3
344	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5c4ocn5)c(n3)-c6ccccc6)CC)c1	5.3
345	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccc(OC)c5N)CC)c1	5.3
346	ONc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.3
347	Oc1c2ccccc2sc1-c3c(nn(c3CC)-c4ccccc4-c5cccc(OCC([O-])=O)c5)-c6ccccc6	5.3
348	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4csc(CC)c4)c(n3)-c5ccccc5)CC)c1	5.3
349	Fc1cc(cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1)C	5.3
350	Fc1c(F)cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.3
351	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(cc(c4)C)C)c(n3)-c5ccccc5)CC)c1	5.3

352	Fc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1N	5.3
353	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(cc5)COC)CC)c1	5.3
354	Clc1c(cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1C)C	5.3
355	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc6ccc(cc6s5)C)CC)c1	5.3
356	OCc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.3
357	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cscc5)CC)c1	5.3
358	FC(F)(F)c1csc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.3
359	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(SC)cc5)CC)c1	5.3
360	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4c(c(c(s4)C)C)C)c(n3)-c5ccccc5)CC)c1	5.3
361	O[C@@H](c1ccc(s1)-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.3
362	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(cc5)C=C)CC)c1	5.3
363	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5COCCc5c4)c(n3)-c6ccccc6)CC)c1	5.3
364	Fc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1NN	5.3
365	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(cc5)C#C)CC)c1	5.3
366	Fc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1N	5.3
367	FC(F)(F)c1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cs1	5.3
368	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccn5)CC)c1	5.3
369	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-n4cc(cc4C)C)c(n3)-c5ccccc5)CC)c1	5.3
370	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc(OC)c(c4)C)c(n3)-c5ccccc5)CC)c1	5.3
371	Clc1cc(F)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.3
372	O=[S@](c1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1)C	5.3
373	SCc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.3
374	Sc1ccc(F)cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.3
375	Fc1c(F)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.2
376	Brc1c[nH]c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.2
377	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5c4OCO5)c(n3)-c6ccccc6)CC)c1	5.2
378	Fc1ccc(s1)-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.2
379	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5c(N)cc[nH]5)CC)c1	5.2
380	Fc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1NC	5.2
381	Oc1c(O)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1O	5.2
382	Oc1c(c(O)ccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.2
383	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5c4ccs5)c(n3)-c6ccccc6)CC)c1	5.2
384	Fc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1CO	5.2
385	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc(CCC#N)c4)c(n3)-c5ccccc5)CC)c1	5.2
386	Clc1cc(OC)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.2
387	Fc1cc(F)c(cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.2
388	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccncc5)CC)c1	5.2
389	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc(OC)c(N)c4)c(n3)-c5ccccc5)CC)c1	5.2
390	Oc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1[N+]([O-])=O	5.2
391	Fc1cc(F)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1O	5.2
392	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc6cnsc6c5)CC)c1	5.2
393	Fc1cc(OC)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.2
394	FC(F)(F)c1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.2
395	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(oc4N)C)c(n3)-c5ccccc5)CC)c1	5.2

396	Fc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)ccc1CC	5.2
397	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(ccc4N)C)c(n3)-c5ccccc5)CC)c1	5.2
398	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5csc(SCC)c5)CC)c1	5.2
399	Clc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1OC	5.2
400	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5cc[nH]c5c4)c(n3)-c6ccccc6)CC)c1	5.2
401	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc(cn4C)C)c(n3)-c5ccccc5)CC)c1	5.2
402	OCc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1O	5.2
403	Oc1cc(cc(O)c1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.2
404	OCc1cc(sc1C)-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.2
405	Fc1c(OC)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.2
406	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc(c4)CSC)c(n3)-c5ccccc5)CC)c1	5.2
407	Oc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc(O)c1C	5.2
408	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cn5ccsc5c4)c(n3)-c6ccccc6)CC)c1	5.2
409	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc6c(c5)c(ns6)C)CC)c1	5.2
410	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5c(c4)cns5)c(n3)-c6ccccc6)CC)c1	5.2
411	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccsc5N)CC)c1	5.2
412	OCc1ccccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.2
413	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cccc5c4cco5)c(n3)-c6ccccc6)CC)c1	5.2
414	Fc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c(O)c1	5.2
415	Oc1ccc([N+]([O-])=O)cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.2
416	ONc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.2
417	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(s5)SCC)CC)c1	5.2
418	O=Cc1cscc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.2
419	Clc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1CC	5.2
420	O=[S@@](c1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1)C	5.2
421	FC(F)c1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.2
422	Clc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c(s1)C	5.2
423	OCCc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.2
424	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5c(N)ccs5)CC)c1	5.2
425	Fc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)ccc1CO	5.2
426	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(c(N)c5)C)CC)c1	5.2
427	[O-][N+](=O)c1ccccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.2
428	OCc1cc(N)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.2
429	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5c(CCS5)c4)c(n3)-c6ccccc6)CC)c1	5.2
430	Oc1c([N+]([O-])=O)cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.2
431	Fc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.2
432	OCc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.2
433	Clc1cc(O)c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1C	5.1
434	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cscc5N)CC)c1	5.1
435	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)C(CC)=C)CC)c1	5.1
436	Oc1c(O)c(OC)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.1
437	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccc(c5)C#N)CC)c1	5.1
438	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5C=C)CC)c1	5.1
439	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(s5)COC)CC)c1	5.1

440	[O-][N+](=O)c1c(cccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.1
441	Clc1c(OC)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.1
442	Fc1cc(F)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1N	5.1
443	Oc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1N	5.1
444	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(s5)OC)CC)c1	5.1
445	Clc1cc(F)c(N)cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.1
446	Fc1cc(F)ccc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.1
447	Fc1cc(F)c(N)cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.1
448	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4c[nH]c5c4ccs5)c(n3)-c6ccccc6)CC)c1	5.1
449	Oc1c2ccoc2ccc1-c3c(nn(c3CC)-c4ccccc4-c5cccc(OCC([O-])=O)c5)-c6ccccc6	5.1
450	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(cc5C)C)CC)c1	5.1
451	Clc1c(Cl)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1	5.1
452	OCc1c(OC)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.1
453	Fc1c(F)c(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)ccc1C	5.1
454	Fc1c(SC)ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.1
455	FC(F)(F)c1ccc(s1)-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.1
456	Fc1c(OC)c(F)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.1
457	Clc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1N	5.1
458	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5c(CCO5)c4)c(n3)-c6ccccc6)CC)c1	5.1
459	Fc1cccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1C	5.1
460	Oc1c(O)c(O)c(N)cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.1
461	Fc1c(O)c(F)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.1
462	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccncc5C)CC)c1	5.1
463	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5c(c4)ccs5)c(n3)-c6ccccc6)CC)c1	5.1
464	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc6ccncc6s5)CC)c1	5.1
465	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccc(OCC=C)cc5)CC)c1	5.1
466	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5c(NCCC5)c4)c(n3)-c6ccccc6)CC)c1	5.1
467	Fc1cc(N)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.1
468	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4c(sc(CC)c4)N)c(n3)-c5ccccc5)CC)c1	5.1
469	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5c(c4)COCO5)c(n3)-c6ccccc6)CC)c1	5.1
470	Oc1cc(O)cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1	5.1
471	Fc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc(N)c1C	5.0
472	Oc1cc2c(cc1-c3c(nn(c3CC)-c4ccccc4-c5cccc(OCC([O-])=O)c5)-c6ccccc6)cco2	5.0
473	Oc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1O	5.0
474	Fc1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c(N)c1	5.0
475	S=C1C=C(SS1)c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.0
476	[O-][N+](=O)c1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)ccc1C	5.0
477	Oc1cc(cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c1)C	5.0
478	Fc1cc2cc[nH]c2cc1-c3c(nn(c3CC)-c4ccccc4-c5cccc(OCC([O-])=O)c5)-c6ccccc6	5.0
479	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc5c(nsc5c4)C)c(n3)-c6ccccc6)CC)c1	4.9
480	Fc1cc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)c(O)cc1CC	4.9
481	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)C(C)=C)CC)c1	4.8
482	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc([nH+]c4)N)c(n3)-c5ccccc5)CC)c1	4.8
483	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc[n+](c4)C)c(n3)-c5ccccc5)CC)c1	4.8

484	Oc1cccc([N+]([O-])=O)c1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	4.8
485	[O-][N+](=O)c1ccc(-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)cc1N	4.8
486	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc([nH+]c4)NN)c(n3)-c5ccccc5)CC)c1	4.7
487	Oc1ccc(cc1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C#N	4.7
488	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-[n+]4ccc(cc4)C)c(n3)-c5ccccc5)CC)c1	4.7
489	Oc1c(ccc(O)c1-c2c(nn(c2CC)-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C=O	4.7
490	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-[n+]4ccccc4N)c(n3)-c5ccccc5)CC)c1	4.7
491	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-[n+]4cccc(c4)C)c(n3)-c5ccccc5)CC)c1	4.7
492	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-[n+]4ccccc4)c(n3)-c5ccccc5)CC)c1	4.7
493	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4cc[nH+]c(N)c4)c(n3)-c5ccccc5)CC)c1	4.6
494	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc[nH+]c4NC)c(n3)-c5ccccc5)CC)c1	4.6
495	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc([nH+]c4N)C)c(n3)-c5ccccc5)CC)c1	4.5
496	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4c[nH+]ccc4N)c(n3)-c5ccccc5)CC)c1	4.4
497	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(-c4ccc[nH+]c4N)c(n3)-c5ccccc5)CC)c1	4.4
498	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccc([nH+]5)N)CC)c1	4.3
499	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cc[nH+]c(NC)c5)CC)c1	4.3
500	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5cccc([nH+]5)NN)CC)c1	4.2

Table 6

SMILE and predicted pIC_{50} values for Series 3 derivatives.

N°	SMILES	$_{Pred}pIC_{50}$
1	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(s3)-c4ccccc4)-c5ccccc5)c1	6.5
2	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(N)c(c(c3C)-c4ccccc4)-c5ccccc5)c1	6.3
3	Clc1c(nc(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	6.3
4	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(nc(n3)-c4ccccc4)-c5ccccc5)CC)c1	6.3
5	Fc1c(nc(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	6.2
6	[O-]C(=O)COc1cccc(-c2ccccc2/C(=N/Oc3ccccc3)c4ccccc4Oc5ccccc5)c1	6.1
7	OCCOc1c(c(nc(n1)-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	6.0
8	[O-]C(=O)COc1cccc(-c2ccccc2-n3c4c(c(n3)-c5ccccc5)c(n[nH]4)-c6ccccc6)c1	6.0
9	[O-]C(=O)COc1cccc(-c2ccccc2OC[C@@H](Nc3ccccc3)COc4ccccc4)c1	6.0
10	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(CCC)c(c([nH]3)-c4ccccc4)-c5ccccc5)c1	6.0
11	[O-]C(=O)COc1cccc(-c2ccccc2-c3csc4c(c(nn34)-c5ccccc5)-c6ccccc6)c1	6.0
12	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(c([nH]3)-c4ccccc4)-c5ccccc5)CC)c1	6.0
13	[O-]C(=O)COc1cccc(-c2ccccc2-n3cc(c(c3CC)-c4ccccc4)-c5ccccc5)c1	6.0
14	O=C(O[C@@H]([C@H](OC(=O)C)c1ccccc1)c2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4	5.9
15	Clc1c(OC(=O)C)c(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.9
16	[O-]C(=O)CCc1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.9
17	[O-]C(=O)COc1cccc(-c2ccccc2-n3c4c(c(c(o4)-c5ccccc5)-c6ccccc6)c(n3)C)c1	5.9
18	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(n3C)-c4ccccc4)-c5ccccc5)c1	5.9

19	O=S(=O)(Nc1cc(c(cc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5)C	5.9
20	Clc1c(-c2ccccc2)cc(nc1-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5	5.9
21	O=C(OC)c1c(c(nn1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.9
22	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(n3CC)-c4ccccc4)-c5ccccc5)c1	5.9
23	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(c([nH]3)-c4ccccc4)-c5ccccc5)C)c1	5.9
24	[O-]C(=O)COc1cccc(-c2ccccc2[C@@H]3CN([C@](O3)(c4ccccc4)C)c5ccccc5)c1	5.9
25	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c([nH]3)-c4ccccc4)-c5ccccc5)c1	5.9
26	Brc1cc(c(cc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.9
27	O=C(N)c1c(c(oc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.9
28	O=C([C@H](N(Cc1ccccc1)c2ccccc2)CC)c3ccccc3-c4cccc(OCC([O-])=O)c4	5.9
29	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(c3N)-c4ccccc4)-c5ccccc5)C)c1	5.9
30	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(c(s3)-c4ccccc4)-c5ccccc5)CC)c1	5.9
31	Brc1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)cc(n1-c4ccccc4)-c5ccccc5	5.8
32	[O-]C(=O)COc1cccc(-c2ccccc2-n3cc(c(c3C)-c4ccccc4)-c5ccccc5)c1	5.8
33	Clc1c(c(oc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.8
34	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(s3)-c4ccccc4)-c5ccccc5)c1	5.8
35	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(c4nccn43)-c5ccccc5)-c6ccccc6)c1	5.8
36	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)-c6ccc(cc6)C)c1	5.8
37	[O-]C(=O)COc1cccc(-c2ccccc2OC[C@H](CNc3ccccc3)Cc4ccccc4)c1	5.8
38	O=C([C@H](N(c1ccccc1)C)COc2ccccc2-c3cccc(OCC([O-])=O)c3)c4ccccc4	5.8
39	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(c3)-c4ccccc4)-c5ccccc5)C)c1	5.8
40	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(n3CC=C)-c4ccccc4)-c5ccccc5)c1	5.8
41	O=C(c1cc(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5)C	5.8
42	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(n(c3)-c4ccccc4)-c5ccccc5)c1	5.8
43	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.8
44	[O-]C(=O)COc1cccc(-c2ccccc2-n3c4c(c(c(o4)N)-c5ccccc5)c(n3)-c6ccccc6)c1	5.8
45	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(n3CCCC)-c4ccccc4)-c5ccccc5)c1	5.8
46	O=Cc1c(nc(n1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.8
47	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)-c6ccccc6)c1	5.8
48	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(c3C)-c4ccccc4)-c5ccccc5)C)c1	5.8
49	O=C(Oc1ccccc1)[C@@H](CC(=O)c2ccccc2-c3cccc(OCC([O-])=O)c3)Cc4ccccc4	5.8
50	Br/C(c1ccccc1-c2cccc(OCC([O-])=O)c2)=C(/Nc3ccccc3)c4ccccc4	5.8
51	O=C(Oc1ccccc1)[C@@H]2C(=CCN(C2)c3ccccc3-c4cccc(OCC([O-])=O)c4)c5ccccc5	5.8
52	[O-]C(=O)COc1cccc(-c2ccccc2-n3c4cnn(c4c(n3)-c5ccccc5)-c6ccccc6)c1	5.8
53	[O-]C(=O)COc1cccc(-c2ccccc2/C=C(/C(c3ccccc3)=C/c4ccccc4)C)c1	5.8
54	O=C(OCC)c1c(oc(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.8
55	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(n3C4CC4)-c5ccccc5)-c6ccccc6)c1	5.8
56	O=C(c1c(c(oc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5)C	5.8
57	[O-]C(=O)COc1cccc(-c2ccccc2CS/C(c3ccccc3)=C/c4ccccc4)c1	5.8
58	Oc1c(c(sc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.8
59	O=C(OC)c1c(oc(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.8
60	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(OC)c(c(s3)-c4ccccc4)-c5ccccc5)c1	5.8
61	O=C(OC)[C@@H](c1ccccc1)/C(=N\Nc2ccccc2-c3cccc(OCC([O-])=O)c3)c4ccccc4	5.8
62	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(c(s3)-c4ccccc4)-c5ccccc5)C)c1	5.8

63	O=S(=O)(c1c(-c2ccccc2)cc(nc1-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)C	5.8
64	Clc1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)cc(n1-c4ccccc4)-c5ccccc5	5.8
65	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(N)c(c(n3C)-c4ccccc4)-c5ccccc5)c1	5.8
66	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(n(c3CC)-c4ccccc4)-c5ccccc5)c1	5.8
67	Clc1cc(c(cc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.8
68	[O-][n+]1c(c(nn1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.7
69	[O-]C(=O)COc1cccc(-c2ccccc2-n3ccc4c3cc(n4-c5ccccc5)-c6ccccc6)c1	5.7
70	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(c(o3)-c4ccccc4)-c5ccccc5)CC)c1	5.7
71	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(n(c(c3CC)-c4ccccc4)-c5ccccc5)C)c1	5.7
72	Brc1c(c(sc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.7
73	O=C(OCC)c1c(c(nn1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.7
74	O=C([C@H]([C@@H](Sc1ccccc1)c2ccccc2)C(=O)C)c3ccccc3-c4cccc(OCC([O-])=O)c4	5.7
75	[O-]C(=O)COc1cccc(-c2ccccc2-c3ccc(c(c3OC)-c4ccccc4)-c5ccccc5)c1	5.7
76	Oc1c(c(cc(c1-c2ccccc2)-c3ccccc3)C)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.7
77	O=C(Oc1ccccc1-c2cccc(OCC([O-])=O)c2)[C@H](Sc3ccccc3)Cc4ccccc4	5.7
78	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(n(c3C)-c4ccccc4)-c5ccccc5)c1	5.7
79	Clc1c(nc(c(n1)-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.7
80	Clc1c(c(nn1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.7
81	Brc1c(c(n(c1-c2ccccc2-c3cccc(OCC([O-])=O)c3)C)-c4ccccc4)-c5ccccc5	5.7
82	Oc1c(c(nc(n1)-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.7
83	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(N)c(n(c3C)-c4ccccc4)-c5ccccc5)c1	5.7
84	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(c(n3C)-c4ccccc4)-c5ccccc5)C)c1	5.7
85	[O-]C(=O)COc1cccc(-c2ccccc2-c3c4cccnc4c(c(n3)-c5ccccc5)-c6ccccc6)c1	5.6
86	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(n3)-c4ccccc4)-c5ccccc5)CC#N)c1	5.6
87	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(OC)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.6
88	Oc1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)ccc(c1-c4ccccc4)-c5ccccc5	5.6
89	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(c(c(n3)-c4ccccc4)-c5ccccc5)C)C)c1	5.6
90	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(OCC)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.6
91	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(OC)nc(c(n3)-c4ccccc4)-c5ccccc5)c1	5.6
92	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(nc(c(n3)-c4ccccc4)-c5ccccc5)C)c1	5.6
93	[O-]C(=O)COc1cccc(-c2ccccc2OCC(Oc3ccccc3)Oc4ccccc4)c1	5.6
94	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(nc(c(n3)-c4ccccc4)-c5ccccc5)C(C)C)c1	5.6
95	Clc1cc(-c2ccccc2-c3cccc(OCC([O-])=O)c3)c(OC)c(c1-c4ccccc4)-c5ccccc5	5.6
96	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(N)c(n(c3)-c4ccccc4)-c5ccccc5)c1	5.6
97	O=S(=O)(N([C@H](COc1ccccc1-c2cccc(OCC([O-])=O)c2)C)c3ccccc3)c4ccccc4	5.6
98	[O-]C(=O)COc1cccc(-c2ccccc2OC[C@H](Oc3ccccc3)Cc4ccccc4)c1	5.6
99	O=C(Nc1c(c(nc(n1)-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5)C	5.6
100	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(n(c(n3)-c4ccccc4)-c5ccccc5)COC)c1	5.6
101	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(cc(c(n3)-c4ccccc4)-c5ccccc5)C)c1	5.6
102	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(o3)-c4ccccc4)-c5ccccc5)c1	5.6
103	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(SC)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.6
104	Oc1cc(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.6
105	O=C(NC)c1c(nc(n1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.6
106	[O-]C(=O)COc1cccc(-c2ccccc2OC[C@@H](Nc3ccccc3)Cc4ccccc4)c1	5.6

107	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(C4CC4)c(c(n3)-c5ccccc5)-c6ccccc6)c1	5.6
108	S=C(N(/N=C/c1ccccc1-c2cccc(OCC([O-])=O)c2)c3ccccc3)c4ccccc4	5.6
109	Clc1c(c(cc(c1C)-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.6
110	[O-]C(=O)COc1cccc(-c2ccccc2-c3ccc(c(c3)-c4ccccc4)-c5ccccc5)c1	5.6
111	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3C4CC4)-c5ccccc5)-c6ccccc6)c1	5.6
112	OC1=C(C(O[C@](O1)(c2ccccc2-c3cccc(OCC([O-])=O)c3)C)c4ccccc4)c5ccccc5	5.6
113	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(SC)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.6
114	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c4c(nccn43)-c5ccccc5)-c6ccccc6)c1	5.6
115	[O-]C(=O)COc1cccc(-c2ccccc2-n3c4c(n5c(c(nc35)-c6ccccc6)-c7ccccc7)cccn4)c1	5.5
116	[O-]C(=O)COc1cccc(-c2ccccc2-c3c4c(nsn4)c(c(c3)-c5ccccc5)-c6ccccc6)c1	5.5
117	[O-]C(=O)COc1cccc(-c2ccccc2N3C[C@@H](C(=N3)c4ccccc4)c5ccccc5)c1	5.5
118	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(OCCC)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.5
119	ON([C@@H](Cc1ccccc1)COc2ccccc2-c3cccc(OCC([O-])=O)c3)c4ccccc4	5.5
120	O=C(N)c1c(nc(n1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.5
121	[O-]C(=O)COc1cccc(-c2ccccc2N3CCC[C@](Nc4ccccc4)(CC3)c5ccccc5)c1	5.5
122	O=C(N)c1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.5
123	O=C(c1c(nc(n1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5)C	5.5
124	OCc1c(oc(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.5
125	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(c(n3)-c4ccccc4)-c5ccccc5)C)c1	5.5
126	O=C(N)c1c(c(nn1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.5
127	O=C(OCC)Cc1c(c(cn1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.5
128	Clc1c(c(sc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.5
129	[O-]C(=O)COc1cccc(-c2ccccc2-c3c4c(CCC4)c(c(n3)-c5ccccc5)-c6ccccc6)c1	5.5
130	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(nc(c(n3)-c4ccccc4)-c5ccccc5)C#N)c1	5.5
131	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(OCC=C)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.5
132	[O-]C(=O)COc1cccc(-c2ccccc2OC[C@@H](N(c3ccccc3)C)c4ccccc4)c1	5.5
133	Sc1cc(c(cc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.5
134	S=C1C(=C(N=C(N1)c2ccccc2-c3cccc(OCC([O-])=O)c3)c4ccccc4)c5ccccc5	5.5
135	[O-]C(=O)COc1cccc(-c2ccccc2C=3NN=C(N(N3)c4ccccc4)c5ccccc5)c1	5.5
136	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(n3CC(C)C)-c4ccccc4)-c5ccccc5)c1	5.5
137	[O-]C(=O)COc1cccc(-c2ccccc2O[C@H]([C@@H](Cc3ccccc3)c4ccccc4)C)c1	5.5
138	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(n3CCC)-c4ccccc4)-c5ccccc5)c1	5.5
139	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(N)cc(c(n3)-c4ccccc4)-c5ccccc5)c1	5.5
140	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(c(o3)-c4ccccc4)-c5ccccc5)C#N)c1	5.5
141	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(cc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.5
142	OCCc1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.5
143	F[C@@]1([C@@H](O)[C@@H](O[C@@H]1c2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4)c5ccccc5	5.5
144	Clc1cc(-c2ccccc2-c3cccc(OCC([O-])=O)c3)cc(c1-c4ccccc4)-c5ccccc5	5.5
145	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(Oc4cnccc4)c(c(n3)-c5ccccc5)-c6ccccc6)c1	5.5
146	Clc1c(c(nc(n1)-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.5
147	[O-]C(=O)COc1cccc(-c2ccccc2-n3c4ccccc4n5c(c(nc35)-c6ccccc6)-c7ccccc7)c1	5.5
148	Clc1cc(nc(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.5
149	[O-]C(=O)COc1cccc(-c2ccccc2N/N=C(\[C@@H](c3ccccc3)C#N)c4ccccc4)c1	5.5
150	[O-]C(=O)COc1cccc(-c2ccccc2N3CC[C@](Oc4ccccc4)(C3)c5ccccc5)c1	5.5

151	Clc1c(N)c(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.5
152	[O-]C(=O)COc1cccc(-c2ccccc2/N=C/C(c3ccccc3)=C/c4ccccc4)c1	5.5
153	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(n(c3CCC)-c4ccccc4)-c5ccccc5)c1	5.5
154	O=C(OC)c1cc(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.5
155	[O-]C(=O)COc1cccc(-c2ccccc2N3CC[C@](Nc4ccccc4)(C3)c5ccccc5)c1	5.5
156	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)C)c1	5.5
157	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(cc3CC#N)-c4ccccc4)-c5ccccc5)c1	5.5
158	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(n(c(n3)-c4ccccc4)-c5ccccc5)C6CC6)c1	5.5
159	Fc1c(c(cc(c1C)-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.5
160	[O-]C(=O)COc1cccc(-c2ccccc2C3=NN([C@@](S3)(c4ccccc4)C)c5ccccc5)c1	5.5
161	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(N)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.5
162	O=Cc1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.5
163	Oc1c(c(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5)C=O	5.5
164	[O-]C(=O)COc1cccc(-c2ccccc2-c3ncc(c(n3)-c4ccccc4)-c5ccccc5)c1	5.5
165	[O-]C(=O)COc1cccc(-c2ccccc2OC[C@@H](Oc3ccccc3)CNc4ccccc4)c1	5.5
166	[O-]C(=O)COc1cccc(-c2ccccc2OC[C@](Nc3ccccc3)(c4ccccc4)C)c1	5.5
167	O=C(OC)c1c(nc(n1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.5
168	Cl/C(c1ccccc1-c2cccc(OCC([O-])=O)c2)=C(/Nc3ccccc3)c4ccccc4	5.5
169	[O-]C(=O)COc1cccc(-c2ccccc2[C@H](N(Cc3ccccc3)c4ccccc4)c5ccco5)c1	5.5
170	Oc1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.5
171	O=C([C@H](N(Cc1ccccc1)c2ccccc2)c3cccs3)c4ccccc4-c5cccc(OCC([O-])=O)c5	5.5
172	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(c(o3)-c4ccccc4)-c5ccccc5)C)c1	5.4
173	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(c(-c4ccccc4)c3)-c5ccccc5)C#C)c1	5.4
174	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(-n4cccc4)c(c(n3)-c5ccccc5)-c6ccccc6)c1	5.4
175	FC(F)(F)Oc1cc(c(cc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.4
176	[O-]C(=O)COc1cccc(-c2ccccc2N[C@H]([C@@H](Oc3ccccc3)c4ccccc4)C)c1	5.4
177	[O-]C(=O)COc1cccc(-c2ccccc2/N=C/[C@@H](Cc3ccccc3)c4ccccc4)c1	5.4
178	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(c(s3)-c4ccccc4)-c5ccccc5)C(C)C)c1	5.4
179	O=C(OC)Cc1c(nc(n1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.4
180	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(-n4cncc4)c(c(n3)-c5ccccc5)-c6ccccc6)c1	5.4
181	[O-]C(=O)COc1cccc(-c2ccccc2N3CCn4c(c(nc34)-c5ccccc5)-c6ccccc6)c1	5.4
182	[O-]C(=O)COc1cccc(-c2ccccc2-c3cnc(c(n3)-c4ccccc4)-c5ccccc5)c1	5.4
183	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(n(c(n3)-c4ccccc4)-c5ccccc5)C)c1	5.4
184	Sc1c(c(nn1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.4
185	Oc1c(c(nn1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.4
186	Clc1c(c(c(c(n1)-c2ccccc2-c3cccc(OCC([O-])=O)c3)C)-c4ccccc4)-c5ccccc5	5.4
187	O=C(c1ccccc1-c2cccc(OCC([O-])=O)c2)/C(=C(\Nc3ccccc3)c4ccccc4)C#N	5.4
188	Oc1ccc(-c2c(c(nn2-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)-c6ccccc6)cc1	5.4
189	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3CCCC)-c4ccccc4)-c5ccccc5)c1	5.4
190	O=C1C(=C(N=C(N1)c2ccccc2-c3cccc(OCC([O-])=O)c3)c4ccccc4)c5ccccc5	5.4
191	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(NCC)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.4
192	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(c(n3)CCC)-c4ccccc4)-c5ccccc5)c1	5.4
193	Fc1cc(c(c(O)c1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.4
194	Sc1c(c(nc(n1)-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.4

195	Oc1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)cc(O)c(c1-c4ccccc4)-c5ccccc5	5.4
196	Clc1cn2c(c(nc2n1-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)-c6ccccc6	5.4
197	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(nc(c(n3)-c4ccccc4)-c5ccccc5)N)c1	5.4
198	O[C@@]1(CN(C[C@@H]1c2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4)c5ccccc5	5.4
199	Clc1cc(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.4
200	Clc1c(O)c(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.4
201	Oc1cc(-c2ccccc2-c3cccc(OCC([O-])=O)c3)cc(c1-c4ccccc4)-c5ccccc5	5.4
202	[O-]C(=O)COc1cccc(-c2ccccc2NCC[C@H](Cc3ccccc3)c4ccccc4)c1	5.4
203	Fc1c(c(c(F)c(N)c1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.4
204	[O-]C(=O)COc1cccc(-c2ccccc2-n3nc(c(n3)-c4ccccc4)-c5ccccc5)c1	5.4
205	Fc1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.4
206	[O-]C(=O)COc1cccc(-c2ccccc2N3CC(=C(C3)c4ccccc4)c5ccccc5)c1	5.4
207	Clc1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)cnc(c1-c4ccccc4)-c5ccccc5	5.4
208	Clc1c(nc(n1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.4
209	O=C(Nc1ccccc1-c2cccc(OCC([O-])=O)c2)[C@@H](Nc3ccccc3)c4ccccc4	5.4
210	O=C(N(c1ccccc1)c2c(Oc3ccccc3-c4cccc(OCC([O-])=O)c4)cccn2)c5ccccc5	5.4
211	Brc1cc(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.4
212	On1c(nc(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.4
213	[O-]C(=O)COc1cccc(-c2ccccc2OCC[C@H](Cc3ccccc3)c4ccccc4)c1	5.4
214	Oc1c(c(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5)C	5.4
215	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(OCC)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.4
216	Cl[C@H]1[C@@H](O[C@@H]([C@H]1c2ccccc2)c3ccccc3)c4ccccc4-c5cccc(OCC([O-])=O)c5	5.4
217	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(n(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.4
218	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c([nH]3)-c4ccccc4)-c5ccccc5)c1	5.4
219	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(CCC)c(c(s3)-c4ccccc4)-c5ccccc5)c1	5.4
220	FC(F)(F)c1cc(nc(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.4
221	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(CCCC)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.4
222	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(OC)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.4
223	Clc1cc(c(c(O)c1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.4
224	Fc1cc(-c2ccccc2-c3cccc(OCC([O-])=O)c3)c(O)c(c1-c4ccccc4)-c5ccccc5	5.4
225	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3CCC)-c4ccccc4)-c5ccccc5)c1	5.4
226	O[C@H]1[C@@H](O[C@@]([C@H]1c2ccccc2)(c3ccccc3)C#C)c4ccccc4-c5cccc(OCC([O-])=O)c5	5.4
227	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(c(s3)-c4ccccc4)-c5ccccc5)C#N)c1	5.4
228	O[C@@H]1[C@@H]([C@H](O[C@]1(c2ccccc2-c3cccc(OCC([O-])=O)c3)C=C)c4ccccc4)c5ccccc5	5.4
229	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(OC)c(c(-c4ccccc4)cc3C)-c5ccccc5)c1	5.4
230	Clc1cc(c(c(F)c1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.3
231	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3C)-c4ccccc4)-c5ccccc5)c1	5.3
232	O=C(N[C@H]1[C@@H](O[C@@H]([C@H]1c2ccccc2)c3ccccc3)c4ccccc4-c5cccc(OCC([O-])=O)c5)N	5.3
233	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(CCC(C)C)c(n(n3)-c4ccccc4)-c5ccccc5)c1	5.3
234	O=S(=O)(N)c1c(oc(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.3
235	[O-]C(=O)COc1cccc(-c2ccccc2-n3cc(c(n3)-c4ccccc4)-c5ccccc5)c1	5.3
236	Brc1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.3
237	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3CC=C)-c4ccccc4)-c5ccccc5)c1	5.3
238	Fc1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)ccc(c1-c4ccccc4)-c5ccccc5	5.3

239	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(c4c3OCO4)-c5ccccc5)-c6ccccc6)c1	5.3
240	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3CC)-c4ccccc4)-c5ccccc5)c1	5.3
241	OCc1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.3
242	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(nc(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.3
243	O=C(N[C@@H](Cc1ccccc1)COc2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4	5.3
244	Fc1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)cc([N+]([O-])=O)c(c1-c4ccccc4)-c5ccccc5	5.3
245	ONC(=N)Cc1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.3
246	O[C@@]1([C@@H](O)[C@@H](O[C@H]1c2ccccc2)Oc3ccccc3-c4cccc(OCC([O-])=O)c4)c5ccccc5	5.3
247	[O-]C(=O)COc1cccc(-c2ccccc2[C@H](N(Cc3ccccc3)c4ccccc4)CC)c1	5.3
248	[O-]C(=O)COc1cccc(-c2ccccc2OC[C@](Cc3ccccc3)(c4ccccc4)C)c1	5.3
249	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(NC)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.3
250	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(c(n3)-c4ccccc4)-c5ccccc5)COC)c1	5.3
251	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(n(n3)-c4ccccc4)-c5ccccc5)c1	5.3
252	[O-]C(=O)COc1cccc(-c2ccccc2/C=C/C(c3ccccc3)=C/c4ccccc4)c1	5.3
253	[O-]C(=O)COc1cccc(-c2ccccc2N3C(=NN(C(=N3)c4ccccc4)c5ccccc5)C)c1	5.3
254	[O-]C(=O)COc1cccc(-c2ccccc2-c3nn(c(n3)-c4ccccc4)-c5ccccc5)c1	5.3
255	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(N)c(c(c3)-c4ccccc4)-c5ccccc5)c1	5.3
256	O=C(OCC)c1c(c(c(n1-c2ccccc2-c3cccc(OCC([O-])=O)c3)C)-c4ccccc4)-c5ccccc5	5.3
257	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(n(c(n3)-c4ccccc4)-c5ccccc5)N)c1	5.3
258	[O-]C(=O)COc1cccc(-c2ccccc2N/C=C(\Nc3ccccc3)c4ccccc4)c1	5.3
259	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(OCC#C)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.3
260	[O-][N+](=O)c1cc(c(c(c1-c2ccccc2)-c3ccccc3)C)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.3
261	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(N)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.3
262	O=C(OCC)c1c(nc(n1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.3
263	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(o3)-c4ccccc4)-c5ccccc5)c1	5.3
264	O=C(N(c1ccccc1)CC(Oc2ccccc2-c3cccc(OCC([O-])=O)c3)=O)c4ccccc4	5.3
265	Clc1c(OC)c(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.3
266	[O-]C(=O)COc1cccc(-c2ccccc2O[C@@H](OC)[C@](Cc3ccccc3)(c4ccccc4)C)c1	5.3
267	[O-]C(=O)COc1cccc(-c2ccccc2C=3C([C@@H](N(N3)c4ccccc4)c5ccccc5)(C)C)c1	5.3
268	Clc1cc(-c2ccccc2-c3cccc(OCC([O-])=O)c3)c(O)c(c1-c4ccccc4)-c5ccccc5	5.3
269	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(cc(c(c3)-c4ccccc4)-c5ccccc5)C)c1	5.3
270	Fc1ccc(-c2c(c(nn2-c3ccccc3-c4cccc(OCC([O-])=O)c4)-c5ccccc5)-c6ccccc6)cc1	5.3
271	Fc1c(O)c(c(cc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.3
272	Oc1cc(nc(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.3
273	S=C1N(N=C(N1c2ccccc2)c3ccccc3)c4ccccc4-c5cccc(OCC([O-])=O)c5	5.3
274	Oc1c(OC)c(nc(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.3
275	Clc1c(Cl)c(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.3
276	[O-]C(=O)COc1cccc(-c2ccccc2CCC(Oc3ccccc3)Oc4ccccc4)c1	5.3
277	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(n3)-c4ccccc4)-c5ccccc5)C#N)c1	5.3
278	[O-]C(=O)COc1cccc(-c2ccccc2-c3ccc(c(n3)-c4ccccc4)-c5ccccc5)c1	5.3
279	[O-][N+](=O)[C@@]1(C[C@H](O[C@H]([C@@H]1c2ccccc2)c3ccccc3)c4ccccc4-c5cccc(OCC([O-])=O)c5)C	5.3
280	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(c(-c4ccccc4)c3)-c5ccccc5)C#N)c1	5.3
281	Brc1c(nc(n1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.3
282	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)-c6cnc(cc6)C)c1	5.3

283	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(OC)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.3
284	O=C(Oc1ccccc1)N(CCOc2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4	5.3
285	Fc1c(c(c(F)c(c1-c2ccccc2-c3cccc(OCC([O-])=O)c3)C)-c4ccccc4)-c5ccccc5	5.2
286	O=C(N(c1ccccc1)C(C(=O)c2ccccc2-c3cccc(OCC([O-])=O)c3)=C)c4ccccc4	5.2
287	[O-]C(=O)COc1cccc(-c2ccccc2SS/C(=N/c3ccccc3)c4ccccc4)c1	5.2
288	[O-]/[N+](=N\C#N)c1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.2
289	OCc1c(nc(n1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.2
290	O=S(=O)(N(c1ccccc1)COc2ccccc2-c3cccc(OCC([O-])=O)c3)c4ccccc4	5.2
291	[O-]C(=O)COc1cccc(-c2ccccc2C=3[C@H]([C@H](N(N3)c4ccccc4)c5ccccc5)CC)c1	5.2
292	[O-]C(=O)COc1cccc(-c2ccccc2C#C[C@@H](Oc3ccccc3)c4ccccc4)c1	5.2
293	[O-]C(=O)COc1cccc(-c2ccccc2[C@@]34CC[C@](O4)([C@H](C3)c5ccccc5)c6ccccc6)c1	5.2
294	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.2
295	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(n(c(n3)-c4ccccc4)-c5ccccc5)C#N)c1	5.2
296	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(N)c(n(n3)-c4ccccc4)-c5ccccc5)c1	5.2
297	Clc1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.2
298	[O-]C(=O)COc1cccc(-c2ccccc2N3CN([C@H](C3)c4ccccc4)c5ccccc5)c1	5.2
299	[O-]C(=O)COc1cccc(-c2ccccc2[C@@H]3CC[C@H]([C@H](O3)Oc4ccccc4)c5ccccc5)c1	5.2
300	Fc1c(c(cc(c1-c2ccccc2)-c3ccccc3)C)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.2
301	[O-][N+](=O)c1cc(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.2
302	O[C@H]([C@@H](c1ccccc1)C(Oc2ccccc2-c3cccc(OCC([O-])=O)c3)=O)c4ccccc4	5.2
303	O=C(OCC)c1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.2
304	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(OC)cc(c(n3)-c4ccccc4)-c5ccccc5)c1	5.2
305	FC(F)(F)c1cc(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.2
306	Fc1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)c(F)cc(c1-c4ccccc4)-c5ccccc5	5.2
307	Fc1ccc(-c2c(nc(n2-c3ccccc3)-c4ccccc4)-c5ccccc5-c6cccc(OCC([O-])=O)c6)cc1	5.2
308	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(c(n3)-c4ccccc4)-c5ccccc5)C)c1	5.2
309	S=C1N(C(c2ccccc2)=CN1c3ccccc3-c4cccc(OCC([O-])=O)c4)c5ccccc5	5.2
310	O[C@H](Cn1c(nc(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5)C	5.2
311	OC[C@@H](N(c1ccccc1)C(=O)c2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4	5.2
312	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(n3)-c4ccccc4)-c5ccccc5)C)c1	5.2
313	O=C(OC)[C@H](Oc1ccccc1-c2cccc(OCC([O-])=O)c2)[C@@H](Oc3ccccc3)c4ccccc4	5.2
314	O=C1C(=C(C(N1c2ccccc2-c3cccc(OCC([O-])=O)c3)=C)c4ccccc4)c5ccccc5	5.2
315	[O-]C(=O)COc1cccc(-c2ccccc2C3=N[C@H]([C@@](S3)(c4ccccc4)C)c5ccccc5)c1	5.2
316	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(Oc4ccccc4)c(c(n3)-c5ccccc5)-c6ccccc6)c1	5.2
317	[O-]C(=O)COc1cccc(-c2ccccc2-c3cn(c(n3)-c4ccccc4)-c5ccccc5)c1	5.2
318	[O-]C(=O)COc1cccc(-c2ccccc2O[C@H]3[C@@H]([C@@H]([C@H](O3)C[N+])c4ccccc4)c5ccccc5)c1	5.2
319	Fc1c(F)c(c(c(O)c1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.2
320	O=C(Oc1ccccc1-c2cccc(OCC([O-])=O)c2)N(Oc3ccccc3)c4ccccc4	5.2
321	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3CC#C)-c4ccccc4)-c5ccccc5)c1	5.2
322	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(cc3NC)-c4ccccc4)-c5ccccc5)c1	5.2
323	[O-]C(=O)COc1cccc(-c2ccccc2N3CC(=C(O3)c4ccccc4)c5ccccc5)c1	5.2
324	FC(F)(F)c1c(c(nn1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.2
325	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(cc(c(n3)-c4ccccc4)-c5ccccc5)C#N)c1	5.2
326	OCCn1c(nc(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.2

327	OC[C@H]1[C@@H](C(=NN1c2ccccc2-c3cccc(OCC([O-])=O)c3)c4ccccc4)c5ccccc5	5.2
328	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3N)-c4ccccc4)-c5ccccc5)c1	5.2
329	[O-]C(=O)COc1cccc(-c2ccccc2C=3[C@H]([C@@H](N(N3)c4ccccc4)c5ccccc5)C)c1	5.2
330	O=C1N(C(c2ccccc2)=CN1c3ccccc3-c4cccc(OCC([O-])=O)c4)c5ccccc5	5.2
331	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(-c4ccccc4)c(n3)COC)-c5ccccc5)c1	5.2
332	O=C(c1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5)C	5.2
333	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(c(n3)-c4ccccc4)-c5ccccc5)C#N)c1	5.2
334	[O-]C(=O)COc1cccc(-c2ccccc2/N=C(/[C@@H](Cc3ccccc3)c4ccccc4)C)c1	5.2
335	[O-]C(=O)COc1cccc(-c2ccccc2C=3C[C@H](N(N3)c4ccccc4)c5ccccc5)c1	5.1
336	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(s3)-c4ccccc4)-c5ccccc5)c1	5.1
337	[O-]C(=O)COc1cccc(-c2ccccc2[C@H]3[C@H](OC(C)C)[C@@H]([C@H](O3)c4ccccc4)c5ccccc5)c1	5.1
338	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3C(C)C)-c4ccccc4)-c5ccccc5)c1	5.1
339	[O-]C(=O)COc1cccc(-c2ccccc2C3=NN([C@@](O3)(c4ccccc4)C)c5ccccc5)c1	5.1
340	[O-][N+](=O)c1c(c(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5)C	5.1
341	Fc1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)cc(F)c(c1-c4ccccc4)-c5ccccc5	5.1
342	[O-]C(=O)COc1cccc(-c2ccccc2NN[C@@H](Cc3ccccc3)c4ccccc4)c1	5.1
343	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3CCOC)-c4ccccc4)-c5ccccc5)c1	5.1
344	[O-]C(=O)COc1cccc(-c2ccccc2[C@@H]3CC(=C(O3)c4ccccc4)c5ccccc5)c1	5.1
345	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3C4CCCCC4)-c5ccccc5)-c6ccccc6)c1	5.1
346	Fc1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)cc(c(c1-c4ccccc4)-c5ccccc5)C	5.1
347	Sc1cc(-c2ccccc2-c3cccc(OCC([O-])=O)c3)cc(c1-c4ccccc4)-c5ccccc5	5.1
348	[O-]C(=O)COc1cccc(-c2ccccc2N3C=C[C@H](C(c4ccccc4)=C3)c5ccccc5)c1	5.1
349	[O-]C(=O)COc1cccc(-c2ccccc2/C=N/[C@@H](Cc3ccccc3)c4ccccc4)c1	5.1
350	Oc1c(nc(c(n1)-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.1
351	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(cc3NCC)-c4ccccc4)-c5ccccc5)c1	5.1
352	FC1(F)[C@@H](O[C@@H]([C@H]1c2ccccc2)c3ccccc3)c4ccccc4-c5cccc(OCC([O-])=O)c5	5.1
353	[O-]C(=O)COc1cccc(-c2ccccc2CS[C@@H](Cc3ccccc3)c4ccccc4)c1	5.1
354	O=C(N)Cc1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.1
355	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(-n4cnc(c4)C)c(c(n3)-c5ccccc5)-c6ccccc6)c1	5.1
356	Oc1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)cc(c(c1-c4ccccc4)-c5ccccc5)C	5.1
357	O=C(N([C@@H](COc1ccccc1-c2cccc(OCC([O-])=O)c2)C)c3ccccc3)c4ccccc4	5.1
358	[O-]C(=O)COc1cccc(-c2ccccc2OCC[C@@H](Oc3ccccc3)c4ccccc4)c1	5.1
359	O=C1C(=C([C@@H](N1c2ccccc2-c3cccc(OCC([O-])=O)c3)C)c4ccccc4)c5ccccc5	5.1
360	O=C1N(C(=C(N1c2ccccc2)c3ccccc3)C)c4ccccc4-c5cccc(OCC([O-])=O)c5	5.1
361	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c(c(-c4ccccc4)c3)-c5ccccc5)C)c1	5.1
362	O=S(=O)(N1C[C@@H](CC[C@H]1c2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4)c5ccccc5	5.1
363	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(N(C)C)c(c(n3)-c4ccccc4)-c5ccccc5)c1	5.1
364	Fc1cc(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.1
365	Clc1c(c(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5)C	5.1
366	[O-]C(=O)COc1cccc(-c2ccccc2-[n+]3cc(c(n3C)-c4ccccc4)-c5ccccc5)c1	5.1
367	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3C(C)(C)C)-c4ccccc4)-c5ccccc5)c1	5.1
368	Fc1ccc(-c2c(nn(c2-c3ccccc3)-c4ccccc4)-c5ccccc5-c6cccc(OCC([O-])=O)c6)cc1	5.1
369	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(SC)c(n(n3)-c4ccccc4)-c5ccccc5)c1	5.1
370	O=C(OC)c1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.1

371	O=C(O[C@@H](Cc1ccccc1)c2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4	5.1
372	Fc1c(c(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5)C	5.1
373	Clc1cc(-c2ccccc2-c3cccc(OCC([O-])=O)c3)c(F)c(c1-c4ccccc4)-c5ccccc5	5.1
374	O=C(Oc1ccccc1-c2cccc(OCC([O-])=O)c2)C3[C@H]([C@H]3c4ccccc4)c5ccccc5	5.1
375	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(n3)-c4ccccc4)-c5ccccc5)Cn6cncn6)c1	5.1
376	[O-]C(=O)COc1cccc(-c2ccccc2[C@H](N(Cc3ccccc3)c4ccccc4)C(C)C)c1	5.1
377	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(n(c(n3)-c4ccccc4)-c5ccccc5)C(C)C)c1	5.1
378	[O-]C(=O)COc1cccc(-c2ccccc2O[C@@H](OC)[C@H](Oc3ccccc3)c4ccccc4)c1	5.1
379	O=C([C@@H](Oc1ccccc1)c2ccccc2)Cc3ccccc3-c4cccc(OCC([O-])=O)c4	5.0
380	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(n3)-c4ccccc4)-c5ccccc5)Cc6ccccc6)c1	5.0
381	Fc1ccccc1-n2c(nc(c2-c3ccccc3)-c4ccccc4)-c5ccccc5-c6cccc(OCC([O-])=O)c6	5.0
382	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(C[N+]C)c(c(o3)-c4ccccc4)-c5ccccc5)c1	5.0
383	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(C(C)C)c(n(n3)-c4ccccc4)-c5ccccc5)c1	5.0
384	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3Nc4ccccc4)-c5ccccc5)-c6ccccc6)c1	5.0
385	O=S(=O)(C([C@@H](c1ccccc1)C(=O)c2ccccc2)(C)C)c3ccccc3-c4cccc(OCC([O-])=O)c4	5.0
386	O=C([C@](O)([C@@H](Nc1ccccc1)c2ccccc2)C)c3ccccc3-c4cccc(OCC([O-])=O)c4	5.0
387	[O-]C(=O)COc1cccc(-c2ccccc2N3CCC(=C(C3)c4ccccc4)c5ccccc5)c1	5.0
388	[O-]C(=O)COc1cccc(-c2ccccc2OCN(c3ccccc3)Cc4ccccc4)c1	5.0
389	O=C(N)c1cc(c(nc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.0
390	Oc1ccc(-n2c(nc(c2-c3ccccc3)-c4ccccc4)-c5ccccc5-c6cccc(OCC([O-])=O)c6)cc1	5.0
391	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3CC(C)C)-c4ccccc4)-c5ccccc5)c1	5.0
392	Fc1c[n+](-c2ccccc2-c3cccc(OCC([O-])=O)c3)cc(c1-c4ccccc4)-c5ccccc5	5.0
393	O=C(OC)Cc1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.0
394	OC[C@@H]1[C@H](O[C@@H]([C@H]1c2ccccc2)c3ccccc3)c4ccccc4-c5cccc(OCC([O-])=O)c5	5.0
395	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(N4CCCC4)c(c(n3)-c5ccccc5)-c6ccccc6)c1	5.0
396	Fc1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)c(F)c(O)c(c1-c4ccccc4)-c5ccccc5	5.0
397	[O-]C(=O)COc1cccc(-c2ccccc2-[n+]3c(nc(c(c3)-c4ccccc4)-c5ccccc5)C)c1	5.0
398	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(c(nn3)-c4ccccc4)-c5ccccc5)C)c1	5.0
399	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3-c4ccccc4)-c5ccccc5)-c6ccccc6)c1	5.0
400	[O-][N+](=O)c1c(c(sc1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	5.0
401	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(C[N+]CC)c(c(o3)-c4ccccc4)-c5ccccc5)c1	5.0
402	[O-]C(=O)COc1cccc(-c2ccccc2N3[C@H]([C@@H](C(=N3)c4ccccc4)c5ccccc5)c6ccc(cc6)C)c1	5.0
403	O=S(=O)(N)c1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	5.0
404	[O-]C(=O)COc1cccc(-c2ccccc2C3=NN([C@H](S3)c4ccccc4)c5ccccc5)c1	5.0
405	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(n3)-c4ccccc4)-c5ccccc5)CCC)c1	5.0
406	[O-]C(=O)COc1cccc(-c2ccccc2[C@H]3CC=C([C@H](O3)c4ccccc4)c5ccccc5)c1	5.0
407	O[C@@]1([C@H](C[C@H]([C@H](O1)c2ccccc2)c3ccccc3)C)c4ccccc4-c5cccc(OCC([O-])=O)c5	5.0
408	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(c(o3)-c4ccccc4)-c5ccccc5)C[N+])c1	5.0
409	S=C(N)c1c(nn(c1-c2ccccc2)-c3ccccc3)-c4ccccc4-c5cccc(OCC([O-])=O)c5	4.9
410	[O-][N+](=O)c1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)cc(c(c1-c4ccccc4)-c5ccccc5)C	4.9
411	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(n(c([n+]3C)-c4ccccc4)-c5ccccc5)C)c1	4.9
412	[O-]C(=O)COc1cccc(-c2ccccc2CON(Cc3ccccc3)c4ccccc4)c1	4.9
413	[O-]C(=O)COc1cccc(-c2ccccc2-n3c(N4CCOCC4)c(c(n3)-c5ccccc5)-c6ccccc6)c1	4.9
414	O=C(Oc1ccccc1-c2cccc(OCC([O-])=O)c2)/C(c3ccccc3)=C/c4ccccc4	4.9

415	[O-][N+](=O)c1c(c(cc(c1-c2ccccc2)-c3ccccc3)C)-c4ccccc4-c5cccc(OCC([O-])=O)c5	4.9
416	[O-]C(=O)COc1cccc(-c2ccccc2-[n+]3ccc(c(c3)-c4ccccc4)-c5ccccc5)c1	4.9
417	[O-][N+](=O)c1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)ccc(c1-c4ccccc4)-c5ccccc5	4.9
418	O=C1C(=C(N=C(SC)N1c2ccccc2-c3cccc(OCC([O-])=O)c3)c4ccccc4)c5ccccc5	4.9
419	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(c(nn3)-c4ccccc4)-c5ccccc5)CC)c1	4.9
420	[O-][N+]1=C(C[C@]([C@@H]1c2ccccc2)(c3ccccc3)C)c4ccccc4-c5cccc(OCC([O-])=O)c5	4.9
421	[O-]C(=O)COc1cccc(-c2ccccc2-c3ccc([n+](c3)-c4ccccc4)-c5ccccc5)c1	4.9
422	[O-]C(=O)COc1cccc(-c2ccccc2OC[C@H](Nc3ccccc3)c4ccccc4)c1	4.9
423	Clc1cc(c(c([N+]([O-])=O)c1-c2ccccc2-c3cccc(OCC([O-])=O)c3)-c4ccccc4)-c5ccccc5	4.9
424	[O-]C(=O)COc1cccc(-c2ccccc2OC[C@H](Cc3ccccc3)c4ccccc4)c1	4.9
425	[O-]C(=O)COc1cccc(-c2ccccc2-n3c[n+](c(-c4ccccc4)c3)-c5ccccc5)c1	4.9
426	[O-]C(=O)COc1cccc(-c2ccccc2N3C[C@H]([C@@H](C3)c4ccccc4)c5ccccc5)c1	4.8
427	[O-]C(=O)COc1cccc(-c2ccccc2C3=C[C@H]([C@@H]([C@H](O3)c4ccccc4)c5ccccc5)C)c1	4.8
428	O=C1C(=C(c2ccccc2)C=NN1c3ccccc3-c4cccc(OCC([O-])=O)c4)c5ccccc5	4.8
429	[O-]C(=O)COc1cccc(-c2ccccc2O[C@H]([C@H](Nc3ccccc3)c4ccccc4)C)c1	4.8
430	Fc1ccc([C@@H]2C(=NN([C@H]2c3ccccc3)c4ccccc4)c5ccccc5-c6cccc(OCC([O-])=O)c6)cc1	4.8
431	[O-][n+]1c(cc(c(c1-c2ccccc2)-c3ccccc3)C)-c4ccccc4-c5cccc(OCC([O-])=O)c5	4.8
432	[O-]C(=O)COc1cccc(-c2ccccc2OC/C(=N/c3ccccc3)c4ccccc4)c1	4.8
433	O=C(C([C@@H](Nc1ccccc1)c2ccccc2)=C)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.8
434	[O-]C(=O)COc1cccc(-c2ccccc2C[C@@H]([N+]C)[C@@H](Oc3ccccc3)c4ccccc4)c1	4.8
435	[O-][n+]1c(-c2ccccc2-c3cccc(OCC([O-])=O)c3)ccc(c1-c4ccccc4)-c5ccccc5	4.8
436	O[C@@](Cc1ccccc1)(c2ccccc2)C(Oc3ccccc3-c4cccc(OCC([O-])=O)c4)=O	4.8
437	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(n3Cc4ccccc4)-c5ccccc5)-c6ccccc6)c1	4.8
438	F[C@@H]1[C@@H](O[C@@H]([C@H]([C@H]1O)c2ccccc2)c3ccccc3)c4ccccc4-c5cccc(OCC([O-])=O)c5	4.8
439	[O-]C(=O)COc1cccc(-c2ccccc2[C@H]3C=C[C@@H]([C@H](O3)c4ccccc4)c5ccccc5)c1	4.8
440	Fc1ccc(-n2c(nc(c2-c3ccccc3)-c4ccccc4)-c5ccccc5-c6cccc(OCC([O-])=O)c6)cc1	4.8
441	O=C(N(C[C@@H](Oc1ccccc1)c2ccccc2)C)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.8
442	[O-]C(=O)COc1cccc(-c2ccccc2/C=C/[C@H](Cc3ccccc3)c4ccccc4)c1	4.7
443	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc(c(c[n+]3C)-c4ccccc4)-c5ccccc5)c1	4.7
444	O=C(NC[C@](Oc1ccccc1)(c2ccccc2)C)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.7
445	[O-]C(=O)COc1cccc(-c2ccccc2-[n+]3ccc(c(n3)-c4ccccc4)-c5ccccc5)c1	4.7
446	S=C(c1ccccc1-c2cccc(OCC([O-])=O)c2)CN(c3ccccc3)C(=O)c4ccccc4	4.7
447	[O-]C(=O)COc1cccc(-c2ccccc2C3=C[C@@H](C4CC4)[C@@H]([C@H](O3)c5ccccc5)c6ccccc6)c1	4.7
448	O=C1C(=C(c2c(scn2)N1c3ccccc3-c4cccc(OCC([O-])=O)c4)c5ccccc5)c6ccccc6	4.7
449	O[C@H]([C@@H](Nc1ccccc1)c2ccccc2)C(=O)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.7
450	F[C@]1(C[C@H](O[C@H]1c2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4)c5ccccc5	4.7
451	O=C(OC[C@H](Oc1ccccc1)c2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.7
452	O=C(c1ccccc1-c2cccc(OCC([O-])=O)c2)C/C(=N/c3ccccc3)c4ccccc4	4.7
453	O[C@H]1[C@@H]([C@H](O[C@@]1(O)c2ccccc2-c3cccc(OCC([O-])=O)c3)c4ccccc4)c5ccccc5	4.7
454	O=C(C([C@H](Oc1ccccc1)c2ccccc2)=C)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.7
455	[O-]C(=O)COc1cccc(-c2ccccc2-c3nc([n+](s3)-c4ccccc4)-c5ccccc5)c1	4.6
456	[O-]C(=O)COc1cccc(-c2ccccc2[C@@H]3[C@@H](OC)[C@H]([C@@H](O3)c4ccccc4)c5ccccc5)c1	4.6
457	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(C[N+]C(C)(C)C)c(n(n3)-c4ccccc4)-c5ccccc5)c1	4.6
458	Br[C@@H]1[C@@H](O[C@H]([C@@H]1c2ccccc2)c3ccccc3)c4ccccc4-c5cccc(OCC([O-])=O)c5	4.6

459	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(C[C@H]([N+])CC)c(n(n3)-c4ccccc4)-c5ccccc5)c1	4.6
460	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(C[N+]CCC)c(n(n3)-c4ccccc4)-c5ccccc5)c1	4.6
461	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(C[N+]C(C)C)c(n(n3)-c4ccccc4)-c5ccccc5)c1	4.6
462	[O-]C(=O)COc1cccc(-c2ccccc2[C@@H]3C[C@H]([C@@H](O3)c4ccccc4)c5ccccc5)c1	4.6
463	O=C1C(=C(C(=CN1c2ccccc2-c3cccc(OCC([O-])=O)c3)C)c4ccccc4)c5ccccc5	4.6
464	O=C1C(=C(N=CN1c2ccccc2-c3cccc(OCC([O-])=O)c3)c4ccccc4)c5ccccc5	4.6
465	O=C1N(C[C@H](N1c2ccccc2)c3ccccc3)c4ccccc4-c5cccc(OCC([O-])=O)c5	4.6
466	[O-]C(=O)COc1cccc(-c2ccccc2-c3n[n+](c(s3)-c4ccccc4)-c5ccccc5)c1	4.6
467	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(CC[N+]C)c(n(n3)-c4ccccc4)-c5ccccc5)c1	4.6
468	O=C(N([C@H](Cc1ccccc1)c2ccccc2)C)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.6
469	[O-]C(=O)COc1cccc(-c2ccccc2[C@H]3CC[C@@H]([C@H](O3)c4ccccc4)c5ccccc5)c1	4.6
470	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(n3)-c4ccccc4)-c5ccccc5)C[N+]C)c1	4.6
471	O[C@@H]([C@H](Cc1ccccc1)c2ccccc2)C(=O)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.5
472	[O-]C(=O)COc1cccc(-c2ccccc2-c3c([C@@H]([N+])C)c(n(n3)-c4ccccc4)-c5ccccc5)c1	4.5
473	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(C[N+]C4CC4)c(n(n3)-c5ccccc5)-c6ccccc6)c1	4.5
474	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(n3)-c4ccccc4)-c5ccccc5)C[N+])c1	4.5
475	O=C(NC/C(=N/c1ccccc1)c2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.5
476	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(C[N+]CC)c(n(n3)-c4ccccc4)-c5ccccc5)c1	4.5
477	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(n3)-c4ccccc4)-c5ccccc5)C[C@H]([N+])C)c1	4.5
478	O=C1C(=C(c2ccccc2)C=CN1c3ccccc3-c4cccc(OCC([O-])=O)c4)c5ccccc5	4.5
479	O=C(C[C@H](Cc1ccccc1)c2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.5
480	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc([n+](c(n3)-c4ccccc4)-c5ccccc5)C)c1	4.5
481	O=C(C[C@H](Oc1ccccc1)c2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.5
482	O=C(N[C@H]([C@H](Oc1ccccc1)c2ccccc2)C)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.5
483	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(n3)-c4ccccc4)-c5ccccc5)CC[N+])c1	4.5
484	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(n3)-c4ccccc4)-c5ccccc5)CC(N)=[N+])c1	4.5
485	O=C1[C@@H](S[C@H](N1c2ccccc2)c3ccccc3)c4ccccc4-c5cccc(OCC([O-])=O)c5	4.4
486	[O-]C(=O)COc1cccc(-c2ccccc2-c3ccc([n+](n3)-c4ccccc4)-c5ccccc5)c1	4.4
487	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc(c([n+](n3)-c4ccccc4)-c5ccccc5)C)c1	4.4
488	O=C([C@H]([C@H](Oc1ccccc1)c2ccccc2)C)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.4
489	O=C1C(=C(N=C(N1c2ccccc2-c3cccc(OCC([O-])=O)c3)C)c4ccccc4)c5ccccc5	4.4
490	O=S(=O)(C/C(=N/c1ccccc1)c2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.4
491	O=C1C(=C(c2ccccc2)C=C(N1c3ccccc3-c4cccc(OCC([O-])=O)c4)C)c5ccccc5	4.3
492	[O-]C(=O)COc1cccc(-c2ccccc2-c3c(c(n(n3)-c4ccccc4)-c5ccccc5)C(N)=[N+])c1	4.3
493	O=C(C[C@H](Nc1ccccc1)c2ccccc2)c3ccccc3-c4cccc(OCC([O-])=O)c4	4.2
494	O=C(c1ccccc1-c2cccc(OCC([O-])=O)c2)/C=C\N(Oc3ccccc3)c4ccccc4	4.2
495	OC1=CC(=C(C(=O)N1c2ccccc2-c3cccc(OCC([O-])=O)c3)c4ccccc4)c5ccccc5	4.2
496	[O-]C(=O)COc1cccc(-c2ccccc2-c3cc([n+](c(n3)-c4ccccc4)-c5ccccc5)N)c1	4.2
497	O=C1C(=C(C[C@H](N1c2ccccc2)c3ccccc3)C)c4ccccc4-c5cccc(OCC([O-])=O)c5	4.0
498	O=C(N(Cc1ccccc1)c2ccccc2)[C@@H](c3ccccc3-c4cccc(OCC([O-])=O)c4)CCC	3.9
499	O=C1C(c2ccccc2-c3cccc(OCC([O-])=O)c3)=CC=C(N1c4ccccc4)c5ccccc5	3.9
500	O=C(N(Cc1ccccc1)c2ccccc2)[C@@H](c3ccccc3-c4cccc(OCC([O-])=O)c4)CC	3.8

Table 7

SMILE and predicted pIC_{50} values for Series 4 derivatives.

N°	SMILES	$_{Pred}pIC_{50}$
1	[O-]C(=O)Cc1cn(nn1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	6.3
2	[O-]C(=O)Nc1c2c(sn1)ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)c2	6.3
3	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1[C@H](O)C([O-])=O	6.3
4	O=C(N1CCc2ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc21)CC([O-])=O	6.3
5	O=C(OC)c1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1OCC([O-])=O	6.3
6	O=C(OCC([O-])=O)N1CCC[C@H]1Cc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	6.3
7	O=C(N1[C@H](CC[C@@H](C1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C)CC([O-])=O	6.2
8	O=C(c1c(cc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)C)CC([O-])=O	6.2
9	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1CC([O-])=O	6.1
10	O=S(=O)(NC([O-])=O)c1ccc(s1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	6.1
11	Oc1cc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1CC([O-])=O)C	6.1
12	[O-]C(=O)Cn1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ccc2cn1	6.1
13	O=S(=O)(CC([O-])=O)c1nc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cs1	6.1
14	Oc1ccc(S(=O)(=O)NC([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	6.1
15	O=C(N)c1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1NCC([O-])=O	6.1
16	Clc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1OCC([O-])=O	6.1
17	O=S(=O)(NC([O-])=O)c1c(N)ccc(c1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	6.1
18	O=C(NCC([O-])=O)CCNc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	6.1
19	O=C(N1C[C@H](S[C@@H](C1)C)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	6.0
20	[O-]C(SSCCCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=O	6.0
21	Oc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1CC([O-])=O	6.0
22	O=C(SC([O-])=O)c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	6.0
23	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1/C=C\C([O-])=O	6.0
24	Fc1cc(F)c(cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	6.0
25	O=C1COc2ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc2N1CC([O-])=O	6.0
26	[O-]C(=O)[C@@H]1[C@@H](O1)CCc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	6.0
27	[O-]C(=O)CC(Oc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)(C)C	6.0
28	O=C(N1CCC[C@@H](C1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	6.0
29	O=C(N1C[C@H](C[C@@H](C1)C)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	6.0
30	[O-][N+](=O)c1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1OCC([O-])=O	6.0
31	O=C1CCc2ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc2N1CC([O-])=O	6.0
32	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1OCC([O-])=O	6.0
33	O=S(=O)(NC([O-])=O)c1cccc(c1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.9
34	O=C(c1cc(n(c1)C)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.9
35	Clc1ccc(SCC([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.9
36	O=S(=O)(c1c(ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)CC([O-])=O	5.9
37	[O-]C(=O)Cc1nnnn1-c2cccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)c2	5.9
38	[O-]C(=O)CSc1c(ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.9
39	Fc1ccc(S(=O)(=O)CC([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.9
40	[O-]C(=O)/C=C\c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.9
41	[O-]C(=O)COc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccc1C(C)(C)C	5.9
42	Fc1cc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1NC([O-])=O)C	5.9

43	Fc1ccc(CNC([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.9
44	O[C@@H](CSc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.9
45	[O-]C(=O)CSc1nc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cs1	5.9
46	Fc1ccc(cc1S(=O)(=O)CC([O-])=O)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.9
47	[O-]C(SSc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)=O	5.9
48	[O-]C(=O)CSc1ccc(o1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.9
49	O=[S@@](c1ccc(o1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.9
50	[O-]C(=O)COc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	5.8
51	O=C1CSc2ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc2N1CC([O-])=O	5.8
52	[O-]C(=O)COCc1ccc(o1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.8
53	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1SCC([O-])=O	5.8
54	[O-]C(=O)CSc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.8
55	[O-]C(=O)Cc1cccc2ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc21	5.8
56	[O-]C(=O)CCOCC(c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=C	5.8
57	[O-]C(=O)CCOCC#Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.8
58	Clc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1COC([O-])=O	5.8
59	[O-]C(=O)COc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccc1C(C)C	5.8
60	O=C(c1c(ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)CC([O-])=O	5.8
61	[O-]C(Sc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccn1)=O	5.8
62	O=[S@](Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CCC([O-])=O	5.8
63	O=S(=O)([C@H](c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CCC([O-])=O	5.8
64	[O-]C(=O)C/C=C(/CCCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.8
65	[O-]C(=O)Cc1nccc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.8
66	O=C(N(CC([O-])=O)C)c1csc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.8
67	Clc1c(cc(s1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C(=O)CC([O-])=O	5.8
68	O/C(c1cccn1CC([O-])=O)=C\c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.8
69	O=S(=O)(NCC([O-])=O)Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.8
70	O=S(=O)(NC([O-])=O)c1ccc(o1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.8
71	OCc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1CC([O-])=O	5.8
72	O=C(n1c(cc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C)CC([O-])=O	5.8
73	Fc1cc(OC)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1CC([O-])=O	5.8
74	[O-]C(=O)CO[C@@H]1C[C@@H](C=C(O1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	5.8
75	O=C1[C@@H](Oc2ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc2N1CC([O-])=O)C	5.8
76	Oc1ccc(cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C(=O)CC([O-])=O	5.8
77	[O-]C(=O)Cc1c(ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.8
78	[O-]C(=O)Cc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccc1NC	5.8
79	Fc1cc(N)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1OCC([O-])=O	5.8
80	Fc1cc2c(N(CC([O-])=O)C(=O)CO2)cc1-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	5.8
81	[O-]C(=O)NCc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccn1	5.8
82	O=C1COc2cc(c(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc2N1CC([O-])=O)C	5.8
83	[O-]C(=O)[C@H](Oc1c(OC)ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.7
84	Oc1c(CCC([O-])=O)cccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.7
85	[O-][N+](=O)c1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1CNC([O-])=O	5.7
86	O=S(=O)(c1cccc(c1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.7

87	O=[S@@](C[C@H](C)C([O-])=O)Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.7
88	[O-]C(=O)COC/C=C/Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.7
89	Clc1cc(F)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1OCC([O-])=O	5.7
90	Clc1cc(nc(OCC([O-])=O)n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.7
91	[O-]C(=O)COc1c(ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C#N	5.7
92	[O-]C(=O)Cc1c(sc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.7
93	O[C@@H](c1c(ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)CC([O-])=O	5.7
94	[O-]C(=O)CN(c1cc(N)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.7
95	[O-]C(=O)Cn1c2c(c(n1)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cccn2	5.7
96	Fc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1N)CC([O-])=O	5.7
97	O=C(c1c(sc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)CC([O-])=O	5.7
98	O=C1N(c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ccc2O1)CC([O-])=O	5.7
99	Fc1ccc(Oc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1CC([O-])=O	5.7
100	O=C(c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c5ccnc(c5)CC([O-])=O	5.7
101	O=C1N(c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ccc2S1)CC([O-])=O	5.7
102	Clc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1N)CC([O-])=O	5.7
103	O=C(OCC([O-])=O)c1cccn1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.7
104	[O-]C(Sc1ccc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)=O	5.7
105	[O-]C(=O)COc1cncc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.7
106	[O-]C(=O)CSc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccn1	5.7
107	[O-]C(=O)Cc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccn1	5.7
108	[O-]C(=O)Cc1cc(Nc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ncn1	5.7
109	Clc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1SCC([O-])=O	5.7
110	[O-]C(=O)Cc1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc(c2on1)C	5.7
111	[O-]C(=O)COCc1cccc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.7
112	O=C(N1CC[C@@H](C1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.7
113	O=S(=O)([C@@H](C)C([O-])=O)c1cccc(c1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.7
114	[O-]C(SSc1c(N)ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)=O	5.7
115	O=C(N(CC([O-])=O)C)c1ccc(s1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.7
116	[O-]C(=O)COCCCSc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.7
117	[O-]C(=O)CN(c1c(OC)ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.7
118	O=S(=O)(NCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)NC([O-])=O	5.7
119	[O-]C(=O)COc1c(cc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)C	5.7
120	[O-]C(Sc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)=O	5.6
121	Clc1cc(OC)c(NCC([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.6
122	Fc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1CSC([O-])=O	5.6
123	Clc1ccc(SC([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.6
124	O=C(N(CC([O-])=O)C)c1c(oc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.6
125	[O-]C(=O)C[C@@H](OC)c1cccc(c1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.6
126	Clc1ccc(N(CC([O-])=O)C)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.6
127	[O-]C(=O)CCc1c(sc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.6
128	O=C(c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c5ccnc(SC([O-])=O)c5	5.6
129	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1C(=O)C(=O)C([O-])=O	5.6
130	O=S(=O)(c1c(N)ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	5.6

131	[O-]C(=O)CN(c1c(ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C#N)C	5.6
132	O=C(N(CC([O-])=O)C)c1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c[nH]1	5.6
133	Oc1ccc(cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.6
134	[O-]C(=O)CCCC1(CC1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.6
135	S=C(SC([O-])=O)NCCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.6
136	[O-]C(=O)Cc1cc2c(ncnc2-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cn1	5.6
137	O=C(OCOCCC([O-])=O)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.6
138	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1[C@@H](NC([O-])=O)C	5.6
139	Cl[C@@]1([C@@](C1)(C)C(OCC([O-])=O)=O)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.6
140	Oc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC([O-])=O	5.6
141	O=S(=O)(n1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ccc2cn1)C([O-])=O	5.6
142	[O-]C(=O)CSC[C@@H](Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.6
143	[O-]C(=O)[C@H]1Cc2c(ccc(c2O1)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)C	5.6
144	Clc1cc(Cl)c(OCC([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.6
145	Oc1cc(nc(n1)CC([O-])=O)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.6
146	[O-]C(=O)CCN1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ccc2CC1	5.6
147	[O-]C(=O)Cc1ccc(SC)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.6
148	Clc1cnc(nc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.6
149	[O-]C(=O)Cc1c2c(on1)ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)c2	5.6
150	[O-]C(=O)Cc1cc(cc(n1)C2CC2)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	5.6
151	[O-]C(=O)Cc1ccc2c(c(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)c([nH]2)C)c1	5.6
152	O=C(c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)[C@@H](C)C([O-])=O	5.6
153	Fc1c(OCC([O-])=O)cccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.6
154	Fc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc([C@H](O)CC([O-])=O)c1	5.6
155	O[C@H](c1ccc(s1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.6
156	[O-]C(=O)COCCCCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.6
157	[O-]C(=O)[C@@H]1C=C(Cc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CO1	5.5
158	O=C(c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC([O-])=O	5.5
159	Fc1ccc(cc1Cc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.5
160	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1COC([O-])=O	5.5
161	Fc1ccc(OCC([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.5
162	[O-]C(=O)Cc1coc2ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc21	5.5
163	[O-]C(=O)CCCCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.5
164	O=C(Oc1ccccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.5
165	[O-]C(=O)Cc1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc(c2on1)CC	5.5
166	[O-]C(=O)CCC#CCCNc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.5
167	[O-]C(=O)Cn1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ccc2o1	5.5
168	[O-]C(SC1=N[C@@H](c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CS1)=O	5.5
169	[O-]C(=O)CN1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ccc2OCC1	5.5
170	O=C(N(CC([O-])=O)C)c1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cn1C	5.5
171	O=[S@@](c1cccc(Oc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	5.5
172	[O-]C(=O)CC1(CC1)CSc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.5
173	[O-]C(=O)Cc1cc(Cc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cs1	5.5
174	Oc1ccc(OCC([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.5

175	[O-]C(=O)Cc1c(/C=C/c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccs1	5.5
176	[O-]C(=O)COc1cncc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.5
177	[O-]C(=O)NCCc1c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccs1	5.5
178	O[C@H](Cc1c(ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)C([O-])=O	5.5
179	O=S(=O)(c1ccc(NN)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	5.5
180	[O-]C(=O)CCc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cs1	5.5
181	[O-]C(=O)Cc1cc2ccoc2c(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)c1	5.5
182	[O-]C(=O)COc1c(cnc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	5.5
183	[O-]C(=O)Cc1ccc2c(c(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)c[nH]2)c1	5.5
184	Brc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC([O-])=O	5.5
185	[O-]C(=O)CO[C@H]1CCC[C@H](C1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.5
186	Fc1c(OCC([O-])=O)ccc(F)c1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.5
187	[O-]C(=O)Cc1cc2c(OCO2)c(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)c1	5.5
188	[O-]C(=O)CN(c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC#C	5.5
189	Clc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1O[C@H](C)C([O-])=O	5.5
190	O=C(OCC([O-])=O)c1c(nsc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	5.5
191	[O-]C(=O)Cc1ccc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC	5.5
192	O=[S@@](c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	5.5
193	Clc1c([C@@H](O)CC([O-])=O)cccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.5
194	[O-]C(=O)CSc1csc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.5
195	FC(F)(F)c1cc(OCC([O-])=O)nc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.5
196	Fc1ccc(cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.5
197	O=C(c1cc(OC)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC([O-])=O	5.5
198	[O-]C(=O)C/C=C\c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.5
199	[O-]C(=O)C/C=C(/Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.5
200	[O-]C(=O)[C@H](Oc1c(ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)C	5.5
201	[O-]C(=O)[C@H](Oc1c(ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)CC	5.5
202	[O-]C(=O)CCc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.5
203	[O-]C(=O)Cn1ccc2ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc21	5.5
204	[O-]C(=O)Cc1cnc2ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cn21	5.5
205	O=S(=O)(N1C[C@H](C[C@H](C1)C)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C([O-])=O	5.5
206	[O-]C(=O)C/C(=C/CCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.5
207	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1CNC([O-])=O	5.5
208	[O-]C(=O)/C=N/Oc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.5
209	[O-]C(=O)Cc1cccc(Nc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.5
210	[O-]C(=O)Cc1ccc(OC)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.5
211	Oc1c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc(cc1C(C)C)CC([O-])=O	5.5
212	Clc1ccc(OCC([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.5
213	[O-]C(=O)CN(CC)c1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.5
214	[O-]C(=O)C/C=C(/C)C#Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.5
215	O=S(=O)(NCC([O-])=O)c1c(n[nH]c1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	5.5
216	[O-]C(=O)CN1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ccc2NCC1	5.5
217	Oc1cc(N(CC([O-])=O)C)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.5
218	[O-]C(Sc1cncc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)=O	5.4

219	[O-]C(=O)Cc1ccc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.4
220	[O-]C(=O)COc1ccnc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.4
221	O=S(=O)(c1cc(N)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	5.4
222	[O-]C(=O)CO[C@H](COc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.4
223	Fc1cc(OCC([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.4
224	Clc1c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc(OCC([O-])=O)cn1	5.4
225	[O-]C(=O)C[C@@H]1CCC[C@H](C1)Cc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.4
226	[O-]C(=O)[C@@H]1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ccc2[C@H](C1)C	5.4
227	[O-]C(=O)CSCC1(CC1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.4
228	O=C(NCCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.4
229	O=S(=O)(N[C@H](c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CC([O-])=O	5.4
230	[O-]C(=O)Cc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.4
231	O=C(c1nc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cs1)CC([O-])=O	5.4
232	[O-]C(=O)CC#CCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.4
233	Fc1c(NCC([O-])=O)cc(F)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.4
234	[O-]C(=O)[C@@H]1Cc2c(S1)cccc2-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	5.4
235	O=C(OCC([O-])=O)c1ccncc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.4
236	[O-]C(=O)COCCCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.4
237	Fc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1C(OCC([O-])=O)=O	5.4
238	Oc1cc(OCC([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.4
239	[O-]C(=O)[C@]1(Oc2cccc(c2O1)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)C	5.4
240	Fc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1C)CC([O-])=O	5.4
241	Clc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc([C@H](O)CC([O-])=O)c1	5.4
242	[O-]C(=O)N(Cc1ccccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	5.4
243	[O-]C(=O)CSCc1cc(ccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	5.4
244	[O-][N+](=O)C[C@@H](c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	5.4
245	[O-]C(=O)Cc1coc2cc(c(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc21)C	5.4
246	Oc1c(cc(cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O)C	5.4
247	O=C(N(CC([O-])=O)C)c1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cs1	5.4
248	Clc1ccc(cc1Oc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.4
249	O=S(=O)(CC1(CC1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.4
250	[O-]C(=O)CSc1cncc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.4
251	[O-]C(=O)COc1c(N)ccc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.4
252	[O-]C(SSSCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=O	5.4
253	Fc1cnc(NC([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.4
254	Fc1ccc(cc1[C@@H]2[C@@H](C2)C([O-])=O)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	5.4
255	[O-]C(=O)NNc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.4
256	[O-]C(=O)COc1ccc(N)c(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.4
257	[O-][N+](=O)c1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1NCC([O-])=O	5.4
258	[O-]C(=O)CN(c1ccc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)C	5.4
259	[O-]C(=O)COc1csc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.4
260	Brc1ccc(cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.4
261	[O-]C(=O)Cc1ccc(NN)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.4
262	[O-]C(=O)COCCSc1cccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.4

263	[O-]C(=O)COc1ccc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C#N	5.4
264	[O-]C(=O)Cc1ccc2ccn(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)c2c1	5.4
265	Clc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1O)CC([O-])=O	5.4
266	[O-]C(=O)[C@H](Oc1ccc(N)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.4
267	Clc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1NCC([O-])=O	5.4
268	[O-]C(=O)COc1cc(OC)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.4
269	Clc1cc(SCC([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.4
270	Clc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC([O-])=O	5.4
271	[O-]C(=O)Cc1cc(OC)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.4
272	O=[S@](c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC([O-])=O	5.4
273	[O-]C(=O)CN1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ccc2CCC1	5.4
274	[O-]C(=O)[C@@H]1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ccc2CC1	5.4
275	[O-]C(=O)CN(c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.4
276	Clc1ccc(cc1Nc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.4
277	O=S(=O)(NCC([O-])=O)c1ccc(s1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.3
278	Fc1c(NCC([O-])=O)c(F)c(F)c(F)c1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.3
279	[O-]C(=O)CC#C[C@@H](c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.3
280	O=S(=O)(c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	5.3
281	[O-]C(=O)CSc1ccc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.3
282	Fc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1F)CC([O-])=O	5.3
283	Clc1cc(OCC([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.3
284	[O-]C(=O)Cc1nc2n(n1)c(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cs2	5.3
285	O=S(=O)(NC([O-])=O)Cc1ccccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.3
286	Fc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1O)CC([O-])=O	5.3
287	Fc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C(=O)CC([O-])=O	5.3
288	[O-]C(=O)[C@H]1CCOc2cc(c(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc21)C	5.3
289	FC(F)(F)c1cc(OCC([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.3
290	[O-]C(=O)COc1c(ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1C)C	5.3
291	Oc1cc2CCC[C@@H](c2cc1-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)C([O-])=O	5.3
292	Clc1cc(O/N=C/C([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.3
293	[O-]C(=O)CCC#CCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.3
294	[O-]C(=O)Cc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.3
295	[O-]C(=O)CN(CC)c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.3
296	Fc1ccc(O[C@H](C)C([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.3
297	[O-]C(=O)CC(CSc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=C	5.3
298	[O-]C(=O)COCc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.3
299	[O-]C(=O)/N=N/Cc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.3
300	O=S(=O)(c1ccc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC)C([O-])=O	5.3
301	[O-]C(=O)[C@@H]1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc(c2OCC1)C	5.3
302	[O-]C(=O)[C@@H]1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ccc2CCC1	5.3
303	O=C(Sc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CCC([O-])=O	5.3
304	O=S(=O)(c1c(O)ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	5.3
305	[O-]C(=O)CCc1csc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.3
306	[O-]C(=O)Cc1c(c2cccc(c2[nH]1)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)C	5.3

307	Clc1ccc(cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.3
308	Fc1cc(O/N=C/C([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.3
309	[O-]C(=O)COc1c(N)ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.3
310	[O-]C(=O)C/C=C\CCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.3
311	[O-]C(OCOc1ccccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)=O	5.3
312	[O-]C(=O)CNc1nccc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.3
313	[O-]C(=O)[C@H](N(c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)C	5.3
314	Oc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1OCC([O-])=O	5.3
315	[O-]C(=O)/C=N/OCCCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.3
316	Clc1cnc(NCC([O-])=O)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.3
317	[O-]C(=O)Cc1ccc2cccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)c2c1	5.3
318	O=S(=O)(c1ccc(N)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	5.3
319	O=S(=O)(N(c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)C([O-])=O	5.2
320	[O-]C(=O)CNc1c(ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.2
321	OC/C(CCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=C/CC([O-])=O	5.2
322	[O-]C(=O)[C@@H]1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ccc2OCC1	5.2
323	[O-]C(=O)Cc1ccc(s1)Oc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.2
324	Fc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc(CCC([O-])=O)c1	5.2
325	O=C(OCC([O-])=O)c1ccoc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.2
326	[O-]C(=O)COc1cnn(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.2
327	[O-]C(=O)CCCC(c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=C	5.2
328	Fc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc(C(=O)N(CC([O-])=O)C)c1	5.2
329	Fc1ccc(S(=O)(=O)C([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.2
330	O=C(N(CC([O-])=O)C)c1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c(s1)C	5.2
331	O=S(=O)(n1ccc2ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc21)C([O-])=O	5.2
332	[O-]C(=O)[C@H]1CCCN1c2cccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)c2	5.2
333	Clc1ccc(S(=O)(=O)C([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.2
334	O=C(OC)[C@@H](Oc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	5.2
335	[O-]C(=O)CNc1ccc(SC)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.2
336	O=S(=O)(NCC([O-])=O)c1c[nH]c(c1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.2
337	[O-]C(OCc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)=O	5.2
338	[O-]C(=O)NCc1cc(OC)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.2
339	O=S(=O)(c1ccc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)C([O-])=O	5.2
340	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1COCC([O-])=O	5.2
341	[O-]C(=O)[C@H]1CCOc2c(cc(cc21)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)CC	5.2
342	[O-]C(OCc1csc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)=O	5.2
343	[O-][N+](=O)c1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC([O-])=O	5.2
344	[O-]C(=O)[C@@H]1c2cc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ccc2SCC1	5.2
345	Fc1ccc(c2c1C[C@@H](O2)C([O-])=O)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	5.2
346	Fc1c(cc(S(=O)(=O)C([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	5.2
347	Clc1cc(O[C@H](C)C([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.2
348	[O-]C(=O)CCc1ccc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C	5.2
349	Clc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1OC)CC([O-])=O	5.2
350	[O-]C(=O)CCc1cncc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.2

351	[O-]C(=O)CN(c1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)C	5.2
352	[O-]C(OCc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cs1)=O	5.2
353	Fc1ccc(NC([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.2
354	Fc1c(CC([O-])=O)cccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.2
355	Oc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc(CCC([O-])=O)c1	5.2
356	[O-]C(SCc1ccc(cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C)=O	5.2
357	Clc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)[C@H](O)C([O-])=O	5.2
358	[O-]C(=O)[C@H](Oc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)CC	5.2
359	Fc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc(CNC([O-])=O)c1	5.2
360	O[C@@H](c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C/C=C\CC([O-])=O	5.2
361	O=S(=O)(CCCOCC([O-])=O)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.1
362	Clc1cc(NCC([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.1
363	O=S(=O)(c1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cs1)C([O-])=O	5.1
364	[O-]C(=O)CCO/C=C/c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.1
365	[O-]C(=O)COCc1ccccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.1
366	[O-]C(=O)CCc1ccnc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.1
367	[O-]C(=O)[C@@H](c1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)C	5.1
368	Fc1cc(NCC([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.1
369	[O-]C(=O)[C@@H](OCC)c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.1
370	[O-]C(=O)[C@H]1Cc2cccc(c2O1)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	5.1
371	O[C@@H](c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC([O-])=O	5.1
372	[O-]C(=O)C/C=C/c1ccccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.1
373	Clc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc(S(=O)(=O)C([O-])=O)c1	5.1
374	[O-]C(=O)CSCSc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.1
375	[O-]C(=O)[C@H](Oc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C(C)C	5.1
376	Fc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1NCCC([O-])=O	5.1
377	O=S(=O)(Nc1c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c(cs1)C)C([O-])=O	5.1
378	Fc1c(F)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc(COC([O-])=O)c1	5.1
379	Fc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc(N([C@@H](C)C([O-])=O)C)c1	5.1
380	Oc1c(CNC([O-])=O)cccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.1
381	Fc1c(NCC([O-])=O)cccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.1
382	[O-]C(SCc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccn1)=O	5.1
383	[O-]C(=O)Cc1nc2c(o1)cccc2-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	5.1
384	Clc1ccc(cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)COC([O-])=O	5.1
385	S=C(Oc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	5.1
386	[O-]C(=O)CNc1c(OC)ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.1
387	O=S(=O)(n1c2ccccc2c(n1)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)C([O-])=O	5.1
388	[O-]C(=O)Cc1cc2cccc(c2[nH]1)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	5.1
389	[O-]C(=O)[C@@H](CC)c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.1
390	[O-]C(OCc1cccc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)=O	5.1
391	O=C(OCCC([O-])=O)[C@@H](c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.1
392	[O-]C(=O)Cc1csc2ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc21	5.1
393	Clc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c6c1nc(o6)CC([O-])=O	5.1
394	Fc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc(S(=O)(=O)C([O-])=O)c1	5.1

395	[O-]C(=O)CNc1c(ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C#N	5.1
396	O=C(Nc1ccsc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.1
397	F[C@@]1(Oc2cccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)c2O1)C([O-])=O	5.1
398	[O-]C(=O)[C@H]1Cc2cc(cc(c2O1)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)C	5.0
399	O=C(c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c5coc(c5)CC([O-])=O	5.0
400	SCc1c(nc(s1)CC([O-])=O)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.0
401	O=S(=O)(c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CCOCC([O-])=O	5.0
402	[O-]C(=O)Cc1nc2cccc(c2[nH]1)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	5.0
403	Clc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1NCCC([O-])=O	5.0
404	[O-]C(=O)CNc1c(c2c(s1)CCC2)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	5.0
405	[O-]C(=O)Cc1nc2cccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)c2o1	5.0
406	[O-]C(OCc1nc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cs1)=O	5.0
407	Fc1cc(NCC([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1OC	5.0
408	[O-]C(=O)CNc1c(N)ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.0
409	O=C(O[C@@H](c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C(C)C)CC([O-])=O	5.0
410	O=C1c2cccc(c2N[C@H](N1)C([O-])=O)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	5.0
411	Fc1ccc(NCC([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.0
412	[O-]C(=O)CNc1ccc(OC)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.0
413	[O-]C(=O)C[C@H]([N+])c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.0
414	Oc1c(OCC([O-])=O)cccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.0
415	O=C(COc1cc(sc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C)C([O-])=O	5.0
416	[O-]C(OCc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)=O	5.0
417	[O-]C(=O)CNc1c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccs1	5.0
418	[O-]C(=O)[C@H](Oc1c([nH+]cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)N)C	5.0
419	[O-]C(=O)CCCc1cc(sc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	5.0
420	[O-]C(=O)Nc1csc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.0
421	[O-]C(=O)CCSSc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.0
422	[O-]C(=O)[C@H]1COc2ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)cc21	5.0
423	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1OCCC([O-])=O	5.0
424	Clc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1CSC([O-])=O	5.0
425	[O-]C(=O)Nc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c(s1)C	5.0
426	Fc1ccc(cc1C2(CC2)C([O-])=O)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	5.0
427	Fc1c(F)c(NCC([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.0
428	Fc1ccc([C@H](CC)C([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.0
429	O=S(=O)(c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)/C=C/CC([O-])=O	5.0
430	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1N[C@@H](C)C([O-])=O	5.0
431	[O-]C(SCCSc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=O	5.0
432	O=[S@](CC1(CC1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.0
433	Clc1cc(c2c(C[C@@H](O2)C([O-])=O)c1)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	5.0
434	Fc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC([O-])=O	5.0
435	[O-]C(=O)[C@H](Oc1ccc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)CC	5.0
436	O=S(=O)(Nc1ccsc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C([O-])=O	5.0
437	Clc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc(COC([O-])=O)c1	5.0
438	[O-]C(=O)COCSc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.9

439	[O-]C(=O)COC[C@@H](Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	4.9
440	O=S(=O)(Nc1ccccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C([O-])=O	4.9
441	[O-]C(=O)COC[C@@H](c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	4.9
442	Fc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc(COC([O-])=O)c1	4.9
443	Fc1c(F)ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1NCCC([O-])=O	4.9
444	O=S(=O)(Nc1c(ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)C([O-])=O	4.9
445	[O-]C(=O)COc1c([nH+]cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)N	4.9
446	O=C(OCC([O-])=O)CSCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.9
447	O=C(c1c(oc(c1)CC([O-])=O)C)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.9
448	Fc1cc([C@@H](C)C([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	4.9
449	S=C(c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c5c(nc(s5)CC([O-])=O)C	4.9
450	O=S(=O)(N1CCC[C@H](C1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	4.9
451	[O-]C(SSSSc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=O	4.9
452	[O-]C(=O)CCC/C(=C\c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	4.9
453	[O-]C(=O)CCC/C=C(/c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	4.9
454	Clc1c(cc(O[C@H](C)C([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	4.9
455	[O-]C(=O)[C@H](Oc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC	4.9
456	Fc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc([C@H](CC)C([O-])=O)c1	4.9
457	O=S(=O)(n1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	4.9
458	Fc1cc(cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)[C@@H](O)C([O-])=O	4.9
459	FC(F)(c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	4.8
460	[O-]C(=O)[C@H](Nc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C#N	4.8
461	[O-]C(=O)Cc1nc2c(ccc(-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)c2[nH]1)C	4.8
462	Fc1c(NS(=O)(=O)C([O-])=O)cccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.8
463	[O-]C(=O)CCCc1ccccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.8
464	[O-]C(=O)Cc1cc2c(o1)cccc2-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	4.8
465	FC(F)(F)c1ccc(NCC([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.8
466	[O-]C(=O)CNc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	4.8
467	Fc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc(NS(=O)(=O)C([O-])=O)c1	4.8
468	Fc1ccc(N[C@@H](C)C([O-])=O)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	4.8
469	Clc1cc(NCC([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1Cl	4.8
470	Oc1c(NS(=O)(=O)C([O-])=O)cccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.8
471	O=S(=O)(Nc1ccc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)C([O-])=O	4.8
472	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc1NS(=O)(=O)C([O-])=O	4.8
473	[O-]C(SCc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cs1)=O	4.7
474	[O-]C(=O)CNc1c(c2c(s1)CCCC2)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	4.7
475	[O-]C(=O)CNc1ccc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)CC	4.7
476	Fc1cccc(NCCC([O-])=O)c1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.7
477	[O-]C(=O)CNc1c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cc(s1)C	4.7
478	[O-]C(=O)[C@H]1Nc2cccc(c2O1)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	4.7
479	Fc1cccc(NS(=O)(=O)C([O-])=O)c1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.7
480	[O-]C(=O)[C@H](c1ccc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C)C#N	4.7
481	O=S(=O)(Nc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)C([O-])=O	4.7
482	[O-][N+](=O)c1cc(NCC([O-])=O)cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	4.7

483	Fc1ccc(c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1)COCC([O-])=O	4.7
484	[O-]C(=O)CNc1cc[nH+]c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	4.6
485	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c(NCCC([O-])=O)c1	4.6
486	Fc1ccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c(CN(C)C([O-])=O)c1	4.6
487	Clc1cccc(NCCC([O-])=O)c1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.6
488	[O-]C(=O)CCNc1cccc(c1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	4.6
489	O=S(=O)(Nc1cc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccn1)C([O-])=O	4.6
490	[O-]C(=O)COCc1ccsc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.6
491	Fc1ccc(CS(=O)(=O)C([O-])=O)cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.6
492	O=S(=O)(Nc1ccc(cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C)C([O-])=O	4.6
493	[O-]C(=O)CCNc1ccc(cc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	4.6
494	[O-]C(=O)C[N+]Cc1c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccs1	4.6
495	Clc1ccc(c(NCCC([O-])=O)c1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.5
496	S=C(Nc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)NCCC([O-])=O	4.5
497	[O-]C(=O)CCNc1ccccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.5
498	Fc1ccc(NCCC([O-])=O)c(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	4.5
499	[O-]C(SSCc1ccccc1-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)=O	4.4
500	[O-]C(=O)[C@H]([N+])c1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	4.4

Table 8

SMILE and predicted pIC_{50} values for Series 5 derivatives.

N°	SMILES	$_{Pred}pIC_{50}$
1	O=C(NC([O-])=O)COC(=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ccs1	6.7
2	[O-]C(=O)c1nnc2n1N=C(c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)CS2	6.5
3	O=C(O[C@H](C)C([O-])=O)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	6.4
4	O=C(N[C@H]1CCC[C@@H]([C@@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CSC([O-])=O	6.4
5	O=C1C(CCC([O-])=O)=CCN1CCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	6.3
6	O=C(N[C@H](CC([O-])=O)C)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ccs1	6.3
7	S/C(NCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=N/C([O-])=O	6.3
8	[O-]C(=O)/N=C(\NCCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)N	6.3
9	O=C(OCC([O-])=O)CS[C@H](n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C	6.2
10	O=C(Nc1ccc(N)cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CCC([O-])=O	6.2
11	O=C(NCCC([O-])=O)c1cccn1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	6.2
12	O=C(NCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)/C=C\C([O-])=O	6.2
13	O=C(OCC([O-])=O)CSCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	6.2
14	O=C(NCCC([O-])=O)c1ccc(N)cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	6.1
15	[O-]C(=O)Cc1cn(nn1)C[C@H]2CC[C@H](O2)n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	6.1
16	O=C(O[C@H](C)C([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c5ccccc5o1	6.1
17	Clc1cccc(NC(=O)CSC([O-])=O)c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	6.1
18	O=C(OCC([O-])=O)Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	6.1

19	O=C(NCC([O-])=O)CSCCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	6.1
20	[O-]C(=O)[C@@H]1c2c(CCO1)cn(n2)CCn3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	6.1
21	Clc1cccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1CC(=O)NCC([O-])=O	6.1
22	O=C(Nc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CCC([O-])=O	6.1
23	O=C(Oc1ccc(cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CCC([O-])=O	6.0
24	O=C(NCCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)nc(s1)N	6.0
25	[O-]C(=O)Cc1ccccc1OCCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	6.0
26	O=C(NCc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ncs1)CC([O-])=O	6.0
27	Brc1ccc(NC(=O)CSC([O-])=O)c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1	6.0
28	O=C(Nc1ccc(cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CCC([O-])=O	6.0
29	[O-]C(=O)[C@@H]1[C@@](O1)(CC[C@H]2[C@](O2)(n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C)C	6.0
30	O=C1C=CC(=NN1CC([O-])=O)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	6.0
31	O=C(NCc1c(cccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CC([O-])=O	6.0
32	O=C(Nc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CSC([O-])=O	5.9
33	[O-]C(Sc1nc(SCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)cc(n1)C)=O	5.9
34	O=C(NCC([O-])=O)CC[C@H](n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C	5.9
35	O=C(N[C@@H]1CCCC[C@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CCC([O-])=O	5.9
36	O=C(OCCC([O-])=O)c1cc(N)ccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.9
37	[O-]C(=O)C[C@@H]1CC(=NO1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.9
38	O=C(NCc1cccnc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.9
39	O=C(N(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C)c4ccnc(OC([O-])=O)c4	5.9
40	[O-]C(=O)CCO[C@H]1CCCC[C@@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.9
41	O=C(NC([O-])=O)[C@H](Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.9
42	[O-]C(=O)Cc1nc(CCCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)cs1	5.9
43	O=C(OC[C@@H]1C=C[C@@H](O1)n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.9
44	Clc1c(N)cc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(c1)C(OCC([O-])=O)=O	5.9
45	O=C(NCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c5ccccc5s1	5.9
46	O=[S@@](CCCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)CCC([O-])=O	5.9
47	O=C(OCC([O-])=O)c1c(cccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.9
48	Fc1cccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1NC(=O)CCC([O-])=O	5.9
49	Fc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(CNC(=O)CC([O-])=O)c1	5.8
50	[O-]C(=O)CCCSCCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	5.8
51	O=C(OCC([O-])=O)c1cc(oc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.8
52	O=C(c1cc(n(c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)C)CSC([O-])=O	5.8
53	O=C(NC([O-])=O)Cc1c[nH]c2cccc(-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c21	5.8
54	Clc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(NC(=O)CSC([O-])=O)c1	5.8
55	O=C(/C=C/Nc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C([O-])=O	5.8
56	[O-]C(=O)[C@@H]1CN(CCO1)c2c3c([nH]cc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ncn2	5.8
57	[O-]C(=O)Cc1ccc2c(c(CCn3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c[nH]2)c1	5.8
58	[O-]C(=O)CCc1nc(CCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)cs1	5.8
59	Oc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)C(OCC([O-])=O)=O	5.8
60	[O-]C(Sc1nc(SCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)sn1)=O	5.8
61	O=C(Nc1c(cccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CSC([O-])=O	5.8
62	Fc1cccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1CC(=O)NCC([O-])=O	5.8

63	Fc1cccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1CNC(=O)CC([O-])=O	5.8
64	O=S(=O)(NC(=O)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C([O-])=O	5.8
65	O=C(Nc1cc(ccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CCC([O-])=O	5.8
66	O=S(=O)(CC([O-])=O)/C=C/c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.8
67	[O-]C(=O)Cc1csc(n1)CCOn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.8
68	O=C(NCc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ccs1)CC([O-])=O	5.8
69	O=C(NCC([O-])=O)Cc1cc(ccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.8
70	O=C(c1cc([nH]c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CSC([O-])=O	5.8
71	Oc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(c1)C(OCC([O-])=O)=O	5.8
72	O=C(NCCC([O-])=O)c1cc(oc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.8
73	O=C(NCC([O-])=O)C[C@@H](Nn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C	5.8
74	Clc1c(Cl)cnc(c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C(OCC([O-])=O)=O	5.8
75	O=C(OCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ccs1	5.8
76	O=C(c1cc(sc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CCC([O-])=O	5.8
77	[O-]C(=O)CCC#Cc1cc(ccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.8
78	[O-]C(=O)Cc1csc(SCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)n1	5.8
79	[O-]C(=O)Cc1csc(NCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)n1	5.8
80	O=C(N[C@@H](c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CC([O-])=O	5.8
81	O=C(NCCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ccs1	5.8
82	O=C(OCC([O-])=O)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.8
83	[O-]C(=O)CCCOc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)cccn1	5.8
84	[O-]C(=O)CSc1cccc(CCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1	5.8
85	O=S(=O)(NCCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)CCC([O-])=O	5.8
86	O=C(NCCC([O-])=O)c1ccc(n1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.7
87	O=C(Nc1cccnc1N(n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CC([O-])=O	5.7
88	Clc1c(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)nn1C)C(=O)NCCC([O-])=O	5.7
89	O=C(OCC([O-])=O)c1cccc(c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.7
90	O=C(NCCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)nc(s1)C	5.7
91	S=C(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)Nc4cccc(c4)CC([O-])=O	5.7
92	[O-]C(=O)CCOCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.7
93	O=C(OCCCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)CCC([O-])=O	5.7
94	O=C(OCCC([O-])=O)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.7
95	O=C(OCC([O-])=O)c1cnn(c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.7
96	O=C(NCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)nc(s1)C	5.7
97	O=C(NCCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ncs1	5.7
98	O=C(N[C@H](C)C([O-])=O)C[N+]1CCCC[C@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.7
99	O=C(OCCOn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)CC([O-])=O	5.7
100	O=C(OCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ncs1	5.7
101	O=C(OCC([O-])=O)c1ccc(N)cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.7
102	Clc1cccc(c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C(OCC([O-])=O)=O	5.7
103	O=C(OCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)nc(s1)C	5.7
104	[O-]C(=O)NC=1C=C(NCCN1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.7
105	Brc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(CNC(=O)CC([O-])=O)c1	5.7
106	O=C(NCc1cccnc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)[C@H](C)C([O-])=O	5.7

107	O=C(NCCC([O-])=O)c1cc(N)cn1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.7
108	O=C(NCc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)cccn1)CC([O-])=O	5.7
109	[O-]C(=O)Cc1csc(n1)COn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.7
110	Fc1cccc(NC(=O)CCC([O-])=O)c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.7
111	O=S(=O)(N[C@@H](c1cc(oc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)C)C([O-])=O	5.7
112	O=C(NCc1c[nH]nc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.7
113	O=C(C(=O)NCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C([O-])=O	5.7
114	O=C(Oc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CCC([O-])=O	5.7
115	O=C(NC([O-])=O)CSc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.7
116	[O-]C(=O)CCCc1nc(Cn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)cs1	5.7
117	O=C(C(=O)NCC[C@H](n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C)C([O-])=O	5.7
118	Fc1cccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1-n5ccc(n5)CC([O-])=O	5.7
119	O=[S@]([C@@H](Cn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C)CC(=O)NC([O-])=O	5.7
120	Clc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)C(OCC([O-])=O)=O	5.7
121	[O-]C(=O)CC/N=C/c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.7
122	Clc1cccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1SCC(=O)NC([O-])=O	5.6
123	[O-]C(=O)Cc1csc(NCCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)n1	5.6
124	O=C(OCC([O-])=O)c1cc(ccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.6
125	Clc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(c1)/C=N/OCC([O-])=O	5.6
126	O=C(OCC([O-])=O)c1cc(N)ccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.6
127	O=C(NCC([O-])=O)c1cccnc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.6
128	Clc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)CC(OCC([O-])=O)=O	5.6
129	O=C(OCC([O-])=O)c1cc(OC)ccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.6
130	O=C(NC([O-])=O)CCc1c(cccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.6
131	[O-]C(Sc1nnc(o1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)=O	5.6
132	O=C1N=C(SC([O-])=O)N=C(SCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)N1	5.6
133	Clc1cccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1COC(=O)CC([O-])=O	5.6
134	Clc1cccc(NC(=O)COC([O-])=O)c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.6
135	O=C(NCCC([O-])=O)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.6
136	Clc1cccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1CNC(=O)CC([O-])=O	5.6
137	[O-]C(Oc1cccc(SCCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)=O	5.6
138	O=C(OCCC([O-])=O)c1ccc(N)cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.6
139	O=C(OCC([O-])=O)c1cccnc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.6
140	O=C(NC(=O)COC([O-])=O)c1cccn1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.6
141	O=C(O[C@@H](C)C([O-])=O)c1ccc(N)cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.6
142	Fc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)CC(=O)NCC([O-])=O	5.6
143	O=C(Nc1cccc(N)c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CCC([O-])=O	5.6
144	O=[S@](CC1(n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)COC1)CCC([O-])=O	5.6
145	O=C(OCCCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)CC([O-])=O	5.6
146	O=C(NCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ncs1	5.6
147	O=C(NCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ccs1	5.6
148	Fc1c(N)cc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)C(OCC([O-])=O)=O	5.6
149	O=C(OCC([O-])=O)c1ccc(OC)cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.6
150	O=C1C(=C(N=C(SCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)N1)CC([O-])=O)C	5.6

151	O=C(OCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)nccn1	5.6
152	[O-]C(=O)Nc1cccc(NCCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1	5.6
153	O=C(NCC([O-])=O)c1csnc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.6
154	O=C(NCC([O-])=O)[C@H](n1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)cc(n1)C)C	5.6
155	O=C(OCCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ccs1	5.6
156	O=S(=O)(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)Nc4nc(CC([O-])=O)cs4	5.6
157	[O-]C(=O)CCc1ccc(o1)[C@H]2C[C@H]2n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.6
158	O=C(OCC([O-])=O)c1ccc(cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.6
159	[O-]C(=O)CCn1nnc(n1)CCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.5
160	O=C(NCc1c(n[nH]c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CC([O-])=O	5.5
161	[O-]C(Oc1cccc(-c2cc(nn2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C#N)c1)=O	5.5
162	[O-]C(=O)Cc1nc(CNn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)cs1	5.5
163	O=C(NCC([O-])=O)[C@H](SCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C	5.5
164	O=C(NCCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)cc(s1)C	5.5
165	[O-]C(=O)c1cccc(Nc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.5
166	Fc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)C(OCC([O-])=O)=O	5.5
167	S=C(Nn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)Nc4nc(CC([O-])=O)cs4	5.5
168	O=C(OCc1c(noc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CC([O-])=O	5.5
169	O=C(NC[C@@H]1CCCC[C@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.5
170	O=C(Nc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(c(s1)C)C)CCC([O-])=O	5.5
171	O=C(NCc1ccc([nH+]c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)N)CC([O-])=O	5.5
172	Clc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)-c5cccc(c5)CC([O-])=O	5.5
173	Brc1ccc(NC(=O)CCC([O-])=O)c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1	5.5
174	O=C(NCc1c(sc(n1)C)-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.5
175	Clc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)-c5nc(SC([O-])=O)n[nH]5	5.5
176	O=S(=O)(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)c4ccccc4C#CCC([O-])=O	5.5
177	Clc1cccc(c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C(=O)NCCC([O-])=O	5.5
178	O=C(Nc1ccsc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CSC([O-])=O	5.5
179	O=C(NCc1cc(oc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CC([O-])=O	5.5
180	Fc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(CC(=O)NCC([O-])=O)c1	5.5
181	O=C(Oc1ccccc1On2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.5
182	S=C1NC(=O)/C(C(=O)N1c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)=C/C([O-])=O	5.5
183	[O-]C(=O)Nc1ccc2ccn(CCn3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c2c1	5.5
184	O=S(=O)(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)NCC#CCC([O-])=O	5.5
185	O=C(c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CSC([O-])=O	5.5
186	O=S(=O)(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)Nc4cccc(c4)CC([O-])=O	5.5
187	[O-]C(=O)Cc1nc(CCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)cs1	5.5
188	[O-]C(=O)Cc1nc(CSn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)cs1	5.5
189	Clc1cccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1CC(OCC([O-])=O)=O	5.5
190	S=C1N=N[C@@H](N1/N=C/c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C([O-])=O	5.5
191	O=C(N1CCO[C@@H](C1)C([O-])=O)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.5
192	[O-]C(OCOc1cccc(Cn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)=O	5.5
193	O=C(Nc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(c(s1)C)C)CSC([O-])=O	5.5
194	Fc1ccc(C(=O)N(n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)cc1NC([O-])=O	5.5

195	[O-]C(Sc1cc(nc(SCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)n1)C)=O	5.5
196	Fc1cccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1CC(OCC([O-])=O)=O	5.5
197	Clc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(c1)C(OCC([O-])=O)=O	5.5
198	O=S(=O)(NCC1(CC1)Cn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C([O-])=O	5.5
199	[O-]C(=O)Cc1cccc(SCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1	5.5
200	[O-]C(=O)COc1ccccc1CCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.4
201	[O-]C(=O)Cc1csc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.4
202	O=S(=O)(NC(=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ccs1)C([O-])=O	5.4
203	O=C(N(C)C([O-])=O)/C=C\c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.4
204	[O-]C(OCCSc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=O	5.4
205	S=C(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)c4ccccc4NC(=O)CC([O-])=O	5.4
206	O=C(NCC1(CC1)Cn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.4
207	O=S(=O)(NCc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ccs1)C([O-])=O	5.4
208	Clc1cncc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1NNC(=O)CC([O-])=O	5.4
209	[O-]C(=O)CC#Cc1ccccc1Nn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.4
210	[O-]C(=O)CC[C@H](SSn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C	5.4
211	O=C(Oc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CSC([O-])=O	5.4
212	[O-]C(=O)CNc1ccn(n1)CCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.4
213	Clc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)C(=O)CSC([O-])=O	5.4
214	O=C1[C@H](SC([O-])=O)CCN1c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.4
215	Clc1ccc(cc1NCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.4
216	[O-]C(=O)CO/N=C(/c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.4
217	O=S(=O)(NCC([O-])=O)CCSn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	5.4
218	[O-]C(=O)Cc1nnc(o1)[C@H](Cn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.4
219	[O-]C(=O)[C@H]1Nc2cccc([C@H]3C[C@@H]3Cn4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)c2O1	5.4
220	O=C(c1cc(sc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CSC([O-])=O	5.4
221	O=C(N[C@@H](CCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C)CC([O-])=O	5.4
222	[O-]C(=O)Cc1nc(no1)CSn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.4
223	O=C(OCC([O-])=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c5ccccc5s1	5.4
224	O=C(c1ccc(cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CSC([O-])=O	5.4
225	O=S(=O)(NCc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)cccn1)C([O-])=O	5.4
226	[O-]C(Oc1cccc(CSn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)=O	5.4
227	S=C(NC(=O)Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C([O-])=O	5.4
228	O=C(Nc1ccccc1N(n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CC([O-])=O	5.4
229	O=C(O[C@H]1C[C@H](CC[C@@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CSC([O-])=O	5.4
230	[O-]C(=O)CO/N=C/c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.4
231	O=S(=O)(N[C@@H](c1cnn(c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)C)C([O-])=O	5.4
232	[O-]C(=O)Nc1ccc2c(c(CCn3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c[nH]2)c1	5.4
233	Clc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(CC(=O)NCC([O-])=O)c1	5.4
234	O=C(N[C@@H](c1cc(oc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)C)CC([O-])=O	5.4
235	[O-]C(=O)CC#CCCCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	5.4
236	[O-]C(=O)Nc1cccc(SCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1	5.4
237	[O-]C(=O)NC=1N(C[C@@H](N1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	5.4
238	O=C([C@@H]1CCCN(C1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C([O-])=O	5.4

239	[O-]C(=O)C/C(=C/CCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C	5.4
240	[O-]C(=O)N/N=C/Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.4
241	O=C(OCCNn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)CC([O-])=O	5.3
242	O=C(OC([O-])=O)CSc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.3
243	[O-]C(=O)c1cnn(Cc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.3
244	[O-]C(=O)Cc1nnc(o1)-c2cc(oc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	5.3
245	S=C(SCC(=O)NCC([O-])=O)n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	5.3
246	Fc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)CNC(=O)CC([O-])=O	5.3
247	O=C(NCCC([O-])=O)c1ccncc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.3
248	O=S(=O)(Cn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)c4cccc(OC([O-])=O)c4	5.3
249	O=C1C=C(N=C(SCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)N1)CC([O-])=O	5.3
250	Fc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)C(=O)CSC([O-])=O	5.3
251	[O-]C(=O)Cc1c(oc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	5.3
252	Fc1ccc(CNS(=O)(=O)C([O-])=O)c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1	5.3
253	[O-]C(=O)Cc1cccc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.3
254	O=S(=O)(Nc1cccc(c1)C([O-])=O)[C@H](n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.3
255	O=C(Oc1c(cccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CCC([O-])=O	5.3
256	[O-]C(=O)[C@@H]1C[N+](Cc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CCO1	5.3
257	O=C(N(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C)c4ccnc(SC([O-])=O)c4	5.3
258	O=C(Nc1cccc(N)c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CSC([O-])=O	5.3
259	O=C(N(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C)c4ccnc(N(C)C([O-])=O)c4	5.3
260	Brc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(C(=O)NCCC([O-])=O)c1	5.3
261	[O-]C(=O)Cc1nc(CCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)co1	5.3
262	[O-]C(=O)Cc1noc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.3
263	O=C(OC[C@@H]1CC=CC[C@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.3
264	O=C(N[C@H](CC([O-])=O)C)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.3
265	O=S(=O)(N[C@H]1CCCC[C@@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.3
266	O=C(N(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)[C@@H](C)C#CCC([O-])=O)C	5.3
267	[O-]C(=O)c1csc(Nc2c(cc(cc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C)C)n1	5.3
268	O=C(NCc1ccc(cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CC([O-])=O	5.3
269	[O-]C(=O)CC#CCSn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	5.3
270	[O-]C(=O)CCSCc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)[nH]cn1	5.3
271	O=S(=O)(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)CCC(=O)NCC([O-])=O	5.3
272	[O-]C(=O)Cc1noc(n1)CCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.3
273	[O-]C(SSSCCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)=O	5.3
274	O=C(N[C@@H](c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)nc(s1)C)C)CC([O-])=O	5.3
275	O=C(N(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C)c4cc(NC([O-])=O)ccc4C	5.3
276	[O-]C(=O)[C@H]1Cc2cccc(c2O1)-c3c(-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)ncc(n3)C	5.3
277	Clc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)C(=O)NCCC([O-])=O	5.3
278	Oc1cccc(c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C(OCC([O-])=O)=O	5.3
279	Fc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(c1)C(OCC([O-])=O)=O	5.3
280	[O-]C(=O)COCCc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ncs1	5.3
281	[O-]C(=O)Cc1noc(n1)CNn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.3
282	O=C(O[C@H](CC([O-])=O)C)c1cccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.3

283	[O-]C(=O)CC#CCOCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	5.3
284	[O-]C(=O)CC#Cc1cc(ccc1Nn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.3
285	[O-]C(=O)Cc1noc(n1)-c2cnn(c2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	5.3
286	[O-]C(=O)CCOCCN(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C	5.3
287	O=S(=O)(N[C@H]1CCC[C@@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.3
288	[O-]C(=O)C/C=C/COCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	5.3
289	[O-]C(Sc1n[nH]c(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)=O	5.3
290	[O-]C(=O)C/C=C/c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.3
291	[O-]C(=O)N(c1cccc(CCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)C	5.3
292	Clc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)-c5nnc(o5)CC([O-])=O	5.3
293	[O-]C(=O)CCC#Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.3
294	[O-]C(Sc1nnc(o1)-c2cccnc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)=O	5.3
295	O=C(N[C@H](CC([O-])=O)C)c1c[nH]nc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.2
296	[O-]C(=O)[C@H]1Cc2cc(cc(c2O1)-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC)C	5.2
297	Fc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)C(=O)NCCC([O-])=O	5.2
298	[O-]C(OCC#Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=O	5.2
299	O=C(N1CC[C@@H](C1)C([O-])=O)c2c(-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccs2	5.2
300	[O-]C(=O)CC#CCCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	5.2
301	Clc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(S(=O)(=O)CCC([O-])=O)c1	5.2
302	O=S(=O)(NNC(=O)c1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ccs1)C([O-])=O	5.2
303	O=C(NC[C@@H](On1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C)CC([O-])=O	5.2
304	O=C(Nc1ccccc1Cn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.2
305	[O-]C(=O)Cc1coc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.2
306	[O-]C(=O)[C@@H]1Cc2c(O1)nccc2-c3ccccc3-n4c(c(c(n4)-c5ccccc5)-c6ccccc6)CC	5.2
307	O=S(=O)(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)n4c(nc5ccc(NC([O-])=O)cc54)N	5.2
308	[O-]C(=O)C/C=C(/CCCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C	5.2
309	Fc1ccc(N2CCC[C@@H](NC([O-])=O)C2)c(-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.2
310	Clc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(/C=N/CCC([O-])=O)c1	5.2
311	[O-]C(=O)CC#Cc1ccccc1Cn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.2
312	O=C(N[C@@H](C)C([O-])=O)Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.2
313	O=S(=O)(N[C@H](Cn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C)CC([O-])=O	5.2
314	Fc1ccc(Nc2cccc(c2)C([O-])=O)c(-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.2
315	[O-]C(SC/C=C(/CCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C)=O	5.2
316	O=C(Nc1ccnn1Cn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.2
317	Fc1cccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1COC(=O)CC([O-])=O	5.2
318	Clc1ccc(nc1CSn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)NC([O-])=O	5.2
319	[O-]C(=O)CC[C@H](SCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C	5.2
320	O=C(N(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)CC#CCC([O-])=O)C	5.2
321	O=C(NCC([O-])=O)C[N+]1CCC[C@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.2
322	[O-]C(=O)CNc1ccccc1SCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.2
323	Fc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(C(=O)NCCC([O-])=O)c1	5.2
324	O=C(OCCC([O-])=O)CSn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	5.2
325	O=C(Nc1cncnc1N(n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CC([O-])=O	5.2
326	O=C(NCCC([O-])=O)c1cc(nn1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.2

327	O=S(=O)(N[C@@H](c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)C([O-])=O	5.2
328	[O-]C(=O)CSSSCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	5.2
329	[O-]C(=O)CCCC[N+]1CCCC[C@@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.2
330	[O-]C(=O)c1cccc(O[C@@H]2CCCC[C@H]2n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.2
331	O=C(NC(=O)CC([O-])=O)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.2
332	[O-]C(=O)Cc1csc(-n2c(ccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C)n1	5.2
333	[O-]C(=O)Cc1cccc(-n2ccnc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.2
334	O=C(Nc1ccccc1Nn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)CC([O-])=O	5.2
335	[O-]C(SCCNc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=O	5.1
336	Clc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(C(=O)NCCC([O-])=O)c1	5.1
337	[O-]C(=O)CCSCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.1
338	[O-]C(=O)Nc1nc(-c2c(cc(cc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C)C)cs1	5.1
339	[O-]C(=O)CSc1c2c(sc(c2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C)ncn1	5.1
340	[O-]C(=O)NCCCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.1
341	[O-]C(SCCOc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=O	5.1
342	[O-]C(=O)CC[N+]C[C@H]1CCCN1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.1
343	Clc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(Cc5nc(cs5)C([O-])=O)c1	5.1
344	Clc1ccc(C(=O)N2CC[C@@H](C2)C([O-])=O)c(-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	5.1
345	Clc1ccc(CNS(=O)(=O)C([O-])=O)c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1	5.1
346	[O-]C(=O)C[C@H]1CCN(C1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.1
347	Fc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(NC(=O)CSC([O-])=O)c1	5.1
348	O=C(NCC([O-])=O)c1ccc(cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.1
349	O=C(NCCC([O-])=O)c1ccc(cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.1
350	O=C(NCCC([O-])=O)c1c(N)cccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.1
351	[O-]C(=O)Cc1nc(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cs1	5.1
352	[O-]C(=O)CC#Cc1ccsc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.1
353	Fc1ccc(Cn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(c1)C#CCC([O-])=O	5.1
354	[O-]C(=O)Nc1nc(CCCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)cs1	5.1
355	[O-]C(=O)CNc1ccccc1COn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.1
356	O=S(=O)(Nn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)c4cc(NC([O-])=O)ccc4C	5.1
357	O=C(NCC([O-])=O)COC(=O)Cn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	5.1
358	[O-]C(=O)Nc1nc(-c2cc(ccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C)cs1	5.1
359	[O-]C(=O)N(c1cccc([C@H](Cn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C#N)c1)C	5.1
360	Fc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(CNS(=O)(=O)C([O-])=O)c1	5.1
361	O=C(NCc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ncs1)NC([O-])=O	5.1
362	[O-]C(=O)CCCCC1=CCC[C@@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.1
363	O=C(N1CC[C@@H](C1)C([O-])=O)c2cccn2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.1
364	O=C(NNCC([O-])=O)c1cccc(c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	5.1
365	[O-]C(=O)C[C@@H]1C([C@@H](C[C@@H](O1)CCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)=C	5.1
366	O=S(=O)(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)Cc4nc(CC([O-])=O)cs4	5.1
367	S=C1N(N=C(O1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)CC([O-])=O	5.1
368	O=C(Cn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)c4cccc(c4)CC([O-])=O	5.1
369	[O-]C(=O)Cc1ccc(o1)C[N+]Cn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.1
370	O=S(=O)(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)CC#CCC([O-])=O	5.1

371	[O-]C(=O)CNc1cccc(Sn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1	5.1
372	[O-]C(=O)Cc1nnc(o1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.1
373	[O-]C(=O)CSc1nnc2n1c(-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cs2	5.1
374	[O-]C(SCCSc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=O	5.1
375	[O-]C(=O)Cc1cccc(C[N+]Cn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1	5.1
376	O=C(OCCC([O-])=O)c1cccnc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.1
377	O=S(=O)(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)c4cc(ccc4C)CC([O-])=O	5.1
378	O=S(=O)(CCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C([O-])=O	5.1
379	[O-]C(=O)Nc1nc(-c2ccc(cc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C)cs1	5.0
380	[O-]C(=O)CSc1c2c(scc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ncn1	5.0
381	[O-]C(=O)CC#CC[N+]1CC[C@@H](n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C1	5.0
382	O=C(NCc1cccn1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)NC([O-])=O	5.0
383	[O-]C(SSCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=O	5.0
384	O=C(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)Cc4nc(CC([O-])=O)cs4	5.0
385	[O-]C(=O)c1ccccc1/C=C/c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.0
386	O=C(N(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C)c4cccc(N(C)C([O-])=O)c4	5.0
387	S=C(N/N=C(/c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)C([O-])=O	5.0
388	[O-]C(=O)CCCSc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)nsn1	5.0
389	O=C(OCCC([O-])=O)c1cc(N)cn1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.0
390	[O-]C(Sc1nnc([nH]1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)=O	5.0
391	Fc1ccc(Nn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(c1)C#CCC([O-])=O	5.0
392	O=S(=O)(CC#Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C([O-])=O	5.0
393	O=S(=O)(c1cccc([C@@H](Nn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)c1)C([O-])=O	5.0
394	S=C(SCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)NCCC([O-])=O	5.0
395	Fc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(c1)C#CCC([O-])=O	5.0
396	[O-]C(=O)Cc1nc(N)c2c(n(nn2)Cn3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)n1	5.0
397	Clc1cccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1Cc5nc(cs5)C([O-])=O	5.0
398	O=C(COC(=O)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C([O-])=O	5.0
399	[O-]C(Sc1nc(ns1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)=O	5.0
400	O=C(N[C@H](c1cc(sc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)C)CC([O-])=O	5.0
401	O=C([C@H]1CN(CCC1)C([O-])=O)c2c(-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccs2	5.0
402	Brc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)C(=O)NCCC([O-])=O	5.0
403	O=C(OCCC([O-])=O)c1cccn1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.0
404	O=C(NCc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ccs1)NC([O-])=O	5.0
405	[O-]C(=O)COc1c2c(sc(c2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C)ncn1	5.0
406	[O-]C(=O)CCCOc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	5.0
407	[O-]C(=O)Cc1ccc(o1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	5.0
408	Brc1cnc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(C(=O)NCCC([O-])=O)c1	4.9
409	[O-]C(=O)CCCC[n+]1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.9
410	[O-]C(=O)[C@H]1CCC[N+](C1)Cc2cccn2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.9
411	Clc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)C(=O)NCC([O-])=O	4.9
412	[O-]C(=O)CCC[N+]([C@@H](Cn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C)C	4.9
413	[O-]C(=O)[C@H]1CCC[N+](C1)Cc2c(-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccs2	4.9
414	Fc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)-c5cncc(c5)CC([O-])=O	4.9

415	Fc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)C#CCCC([O-])=O	4.9
416	[O-]C(=O)Cc1[nH]nc(n1)CCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.9
417	[O-]C(=O)C[N+]1CCc2c(C1)c(N(n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C)ncn2	4.9
418	O=C(CNC(=O)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C([O-])=O	4.9
419	[O-]C(=O)CC/C=C(/CCn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C	4.9
420	[O-]C(=O)Nc1cncc(SCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1	4.9
421	[O-]C(=O)CCCO[C@@H]1CCCC[C@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.9
422	O=C(N1CCC[C@@H](C1)C([O-])=O)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.9
423	O=C([C@@H](Cn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C)c4cccc(c4)C([O-])=O	4.9
424	[O-]C(=O)CC[N+]Cc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.9
425	[O-]C(=O)Cc1ccn(-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	4.9
426	[O-]C(=O)Cn1nnc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.9
427	Clc1cccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1C(=O)NCCC([O-])=O	4.9
428	Clc1c(F)cc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)-c5nnc(o5)CC([O-])=O	4.9
429	[O-]C(=O)Cc1noc(n1)C[N+]2CCC[C@H]2n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.9
430	O=S(=O)(NCC([O-])=O)c1cc(ccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	4.9
431	[O-]C(=O)CCC#Cc1ccsc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.8
432	O=C(NCCC([O-])=O)c1c(cccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	4.8
433	[O-]C(=O)C[N+]1CCC[C@@H](C1)c2c(-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c[nH]n2	4.8
434	O=C(Nc1ccccc1[C@@H](n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CC([O-])=O	4.8
435	[O-]C(=O)[C@@H](c1nc(no1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C	4.8
436	Fc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(c1)C#CCCC([O-])=O	4.8
437	[O-]C(=O)Cc1nnc(SCCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)o1	4.8
438	O=C(OCCOC([O-])=O)CSn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	4.8
439	O=S(=O)(n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)CCSCCC([O-])=O	4.8
440	O=S(=O)(NCC([O-])=O)c1c(oc(c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)C	4.8
441	O=C(OCC(C([O-])=O)=C)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.8
442	Fc1cccc(S(=O)(=O)NCC([O-])=O)c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.8
443	[O-]C(=O)CCCSc1nccn1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.8
444	[O-]C(=O)[C@H]1CCC[N+](C1)Cc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.8
445	O=C(NCCC([O-])=O)[C@H]1CC=CC[C@@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.8
446	O=C1CC[C@@H](CN1Cc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C([O-])=O	4.8
447	Clc1ccc(NC(=O)CSC([O-])=O)c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1	4.8
448	O=C(NCCC([O-])=O)c1cccnc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.8
449	Fc1ccc(C[N+]2CCC[C@@H](C2)C([O-])=O)c(-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	4.8
450	O=C(NCCC([O-])=O)c1cc(N)ccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.8
451	O=C(N1CCC[C@@H](C1)C([O-])=O)c2c(-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)ccs2	4.8
452	[O-]C(=O)/C(=N/OCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	4.8
453	[O-]C(=O)[C@H]1CCC[N+](C1)Cc2c(-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)cco2	4.8
454	[O-]C(=O)Cc1nc(no1)CCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.8
455	Clc1ccc(c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1)CNC(=O)CC([O-])=O	4.8
456	[O-]C(=O)[C@H]1CCC[N+](C1)Cc2ccoc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.8
457	[O-]C(=O)C[N+]CCn1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)cc(n1)C	4.8
458	Fc1ccc(-n2cc(nn2)CC([O-])=O)c(-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	4.8

459	[O-]C(=O)CC[N+](Cc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ccs1)C	4.7
460	O=S(=O)(NCC([O-])=O)c1ccc(cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	4.7
461	O=S(=O)(Nc1cccc([C@@H](n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)c1)C([O-])=O	4.7
462	O/C(c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)=C\S(=O)(=O)C([O-])=O	4.7
463	O=C(NCCC([O-])=O)c1cc(sc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	4.7
464	Clc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(N5CC[C@H](C5)CC([O-])=O)c1	4.7
465	O=S(=O)(NCC([O-])=O)c1c([nH]c(c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)C	4.7
466	O=C(NCc1ccc(n1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C)CC([O-])=O	4.7
467	O=C([C@H]1CSC(=N1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C([O-])=O	4.7
468	O=C(OCc1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)[C@@H](C)C([O-])=O	4.7
469	[O-]C(=O)Cc1nc(no1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.7
470	Brc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(S(=O)(=O)NCC([O-])=O)c1	4.7
471	O=C(NCCC([O-])=O)c1cc(ccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	4.7
472	[O-]C(=O)c1csc(n1)C[N+]2CCCC[C@H]2n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.7
473	Fc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(C(OCCC([O-])=O)=O)c1	4.7
474	Fc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(S(=O)(=O)NCC([O-])=O)c1	4.6
475	Brc1ccc(S(=O)(=O)NCC([O-])=O)c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1	4.6
476	[O-]C(=O)C[N+]CCSSn1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC	4.6
477	O=C(Nc1c(ccs1)C([O-])=O)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.6
478	[O-]C(=O)Cc1noc(n1)[C@H]([N+])CCn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.6
479	O=S(=O)(NCC([O-])=O)c1cccc(N)c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.6
480	[O-]C(=O)CC#CC[N+]1[C@H](CCC[C@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C	4.6
481	O=S(=O)(NCC([O-])=O)c1ccc(N)cc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.6
482	Clc1cccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c1S(=O)(=O)NCC([O-])=O	4.6
483	O=C(NC(=O)NC([O-])=O)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.6
484	O=S(=O)(NCC([O-])=O)c1cccnc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.6
485	[O-]C(=O)C[N+]1CC(Oc2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)C1	4.5
486	Clc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(CNC(=O)CC([O-])=O)c1	4.5
487	Clc1ccc(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)c(S(=O)(=O)NCC([O-])=O)c1	4.5
488	[O-]C(=O)CC[N+]Cc1c(-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)ccs1	4.5
489	[O-]C(=O)CC#CC[N+]1CCCC[C@H]1n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.5
490	Fc1ccc(C[N+]2CC[C@@H](C2)C([O-])=O)c(-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)c1	4.5
491	[O-]C(Sc1[nH]nc(n1)-c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC)=O	4.5
492	O=C(NCCC([O-])=O)C[C@@H](n1c(c(c(n1)-c2ccccc2)-c3ccccc3)CC)C	4.4
493	O=S(=O)(NCC([O-])=O)c1cnccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.4
494	O=C(NC[C@@H](C)C([O-])=O)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.4
495	O=S(=O)(NCC([O-])=O)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.4
496	[O-]C(=O)CCNc1ccccc1Cn2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.4
497	O=S(=O)(N[C@@H](C)C([O-])=O)c1ccccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.4
498	[O-]C(=O)C[N+]1CCO[C@@H](C1)c2ccccc2-n3c(c(c(n3)-c4ccccc4)-c5ccccc5)CC	4.3
499	O=S(=O)(N[C@@H](C)C([O-])=O)c1cnccc1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC	4.2
500	Fc1cccc(c1-n2c(c(c(n2)-c3ccccc3)-c4ccccc4)CC)C(=O)NCCC([O-])=O	4.1

Table 9

SMILE and predicted pIC_{50} values for Series 6 derivatives.

N°	SMILES	$_{Pred}pIC_{50}$
1	[O-]C(SC1=[N+][C@](C[C@@]2(Nc3ccccc3N12)c4ccccc4)(c5ccccc5)C)=O	7.3
2	O=C(NC(C([O-])=O)C([O-])=O)[C@H](Cc1ccccc1)c2ccccc2	7.2
3	S=C(N(Nc1ccccc1)c2ccccc2)CCCC([O-])=O	6.6
4	S=C(NN=C(Cc1ccccc1)Cc2ccccc2)C([O-])=O	6.5
5	O=C([C@@H]1[C@H](O[C@](O1)(c2ccccc2)C)c3ccccc3)[C@H](OC)C([O-])=O	6.5
6	O=C(OC([O-])=O)CS[C@H]1[C@@H](O[C@@H](C1)c2ccccc2)c3ccccc3	6.5
7	[O-]C(=O)NCC[C@@H](c1ccccc1)COc2ccccc2	6.4
8	[O-]C(=O)CC([C@@H]([C@H]([C@H](c1ccccc1)C)c2ccccc2)C)=C	6.4
9	[O-]C(=O)[C@H]1[C@H](OC[C@@H](O1)[C@@H](Cc2ccccc2)c3ccccc3)OC	6.4
10	O=C(N(Cc1ccccc1)Cc2ccccc2)[C@@H](CC([O-])=O)C	6.4
11	O=C1[C@@H](N2C(=O)[C@](O[C@@]2([C@@H]3CCCN13)c4ccccc4)(c5ccccc5)C)CC([O-])=O	6.3
12	[O-]C(=O)/C=C\C[C@H](Cc1ccccc1)c2ccccc2	6.3
13	O=C1C[C@@H]([C@@H]([C@@H]1c2ccccc2)/C=C/[C@H](O)C([O-])=O)c3ccccc3	6.3
14	[O-]C(=O)NC[C@H]1C[C@@H]2CC[C@]1([C@@]2(c3ccccc3)C)c4ccccc4	6.3
15	[O-][N+](=O)c1c(N)cc2c(C[C@H]([C@](O2)(c3ccccc3)C)c4ccccc4)c1C([O-])=O	6.2
16	[O-]C(=O)C(OC[C@H](Cc1ccccc1)c2ccccc2)C([O-])=O	6.2
17	[O-]C(O[C@H](OC)CC/C(c1ccccc1)=C/c2ccccc2)=O	6.2
18	O[C@]1(CCC[C@]2(CC[C@@H](C[C@@]12c3ccccc3)C(C([O-])=O)=C)C)c4ccccc4	6.2
19	Clc1ccc(N(Cc2ccccc2)Cc3ccccc3)cc1C([O-])=O	6.2
20	O=C(OC)[C@@H]1[C@@]2(O1)[C@@H](O[C@@H]([C@@H]2c3ccccc3)c4ccccc4)CC([O-])=O	6.2
21	O[C@@H]1CC(=C[C@H]([C@H]1c2ccccc2)c3ccccc3)C(=O)C([O-])=O	6.2
22	O[C@@H](C[C@H]1[C@@]([C@@H]1c2ccccc2)(c3ccccc3)C)C(=O)C([O-])=O	6.2
23	O[C@H]1[C@@H](C[C@@H](C[C@H]1CC([O-])=O)c2ccccc2)c3ccccc3	6.2
24	[O-]C(=O)[C@H]1C[C@H]1CC[C@@H](Nc2ccccc2)c3ccccc3	6.2
25	O=S(=O)(NC1[C@@]([C@@]1(c2ccccc2)C)(c3ccccc3)C)N(C)C([O-])=O	6.2
26	O=C(N[C@H](Cc1ccccc1)c2ccccc2)[C@H](C(OC)=O)C([O-])=O	6.2
27	O[C@]1([C@@](O[C@@H]([C@]1(O)c2ccccc2)c3ccccc3)(CC([O-])=O)C)C	6.2
28	[O-]C(O[C@H]1C[C@@](Oc2ccccc2)([C@@H](OC)[C@H](O1)C)c3ccccc3)=O	6.1
29	O[C@@H]1[C@H](O[C@H]([C@H]1c2ccccc2)c3ccccc3)[C@H](OC)C([O-])=O	6.1
30	O=C(N(Cc1ccccc1)c2ccccc2)/C=C\[S@](=O)C([O-])=O	6.1
31	O=C(N(Cc1ccccc1)c2ccccc2)[C@@H](S(=O)(=O)C([O-])=O)C	6.1
32	O=C([C@](Nc1ccccc1)(CCCC([O-])=O)C)c2ccccc2	6.1
33	S=C(N1C[C@H](N(C[C@@H]1C)c2ccccc2)c3ccccc3)C([O-])=O	6.1
34	O=C(OCC([O-])=O)N1CC[C@@]1(Cc2ccccc2)c3ccccc3	6.1
35	[O-]C(=O)[C@H](/C=C/[C@@H](C1(CC1)c2ccccc2)c3ccccc3)C	6.1
36	O=C(N1C[C@@H]([C@]([C@@H](C1)C)(C(C)C)c2ccccc2)c3ccccc3)C([O-])=O	6.1
37	[O-]C(OC[C@@H]1C[C@@H]([C@H]1Cc2ccccc2)c3ccccc3)=O	6.1
38	[O-]C(=O)C[C@@H]1/C([C@@H](Oc2ccccc2)[C@@H](O1)c3ccccc3)=C\C#N	6.0
39	O=C(N1C[C@H](OC[C@H]1c2ccccc2)OC([O-])=O)c3ccccc3	6.0
40	OC[C@@H]1[C@H]([C@H]([C@H](O1)CCC([O-])=O)c2ccccc2)c3ccccc3	6.0
41	O=S(=O)(N[C@@H]1CN(C[C@H]1c2ccccc2)c3ccccc3)C([O-])=O	6.0
42	[O-]C(=O)CO[C@H]([C@@H](Nc1ccccc1)Cc2ccccc2)C	6.0

43	O=C(N[C@@H]([C@H](c1ccccc1)C)c2ccccc2)[C@H](C)C([O-])=O	6.0
44	O=C(OC([O-])=O)CO[C@@H](Cc1ccccc1)c2ccccc2	6.0
45	[O-]C(=O)C1(C[C@H]2[C@@H](O1)[C@H]([C@H](CO2)c3ccccc3)c4ccccc4)C([O-])=O	6.0
46	[O-]C(=O)CCSC[C@@H]1[C@@H](C[C@@H](O1)c2ccccc2)c3ccccc3	6.0
47	O=S(=O)(CC[C@H](Oc1ccccc1)Cc2ccccc2)C([O-])=O	6.0
48	[O-]C(=O)[C@@]1(C[C@@H]([C@@H](Cc2ccccc2)c3ccccc3)CCO1)C	6.0
49	O=S(=O)(NC[C@@H]1[C@@H](C[C@@H](O1)c2ccccc2)c3ccccc3)C([O-])=O	6.0
50	[O-]C(=O)c1c(OC)ccc([C@@H](Cc2ccccc2)c3ccccc3)c1	6.0
51	[O-]C(O/N=C/1CN(C[C@@]1(c2ccccc2)C)c3ccccc3)=O	6.0
52	[O-]C(=O)c1c2c(OCO2)cc([C@@H]([C@@H](c3ccccc3)C)c4ccccc4)c1	6.0
53	O[C@H]([C@]1(OC)CC([C@@H]([C@@H](O1)c2ccccc2)c3ccccc3)=C)C([O-])=O	6.0
54	O[C@@H]1CO[C@H]([C@@H](Oc2ccccc2)[C@@H]1c3ccccc3)CCC([O-])=O	6.0
55	[O-]C(=O)CC[C@H]([C@H]([C@H](c1ccccc1)C)c2ccccc2)C	6.0
56	[O-]C(=O)c1ccc(o1)[C@@H](N(C2CC2)c3ccccc3)c4ccccc4	6.0
57	[O-]C(=O)CCCC(Cc1ccccc1)Cc2ccccc2	6.0
58	O[C@H]1[C@H]([C@H](O[C@@H]1[C@H](CCC)C([O-])=O)c2ccccc2)c3ccccc3	5.9
59	O=S(=O)(NC1[C@H](C[C@H]1c2ccccc2)c3ccccc3)C([O-])=O	5.9
60	[O-]C(=O)c1ccc(o1)[C@@H]([C@H](c2ccccc2)C)c3ccccc3	5.9
61	O=C1[C@@]([C@@H](N1c2ccccc2)c3ccccc3)(CCCC([O-])=O)CC	5.9
62	O=C(O[C@H](C=C)C([O-])=O)[C@H]1[C@]([C@H]1c2ccccc2)(c3ccccc3)C	5.9
63	O[C@H]1[C@H](NC([O-])=O)[C@H](C[C@@H]([C@@H]1c2ccccc2)c3ccccc3)C	5.9
64	Br[C@H]1[C@@H](O[C@H]([C@@H]1c2ccccc2)COC([O-])=O)c3ccccc3	5.9
65	[O-]C(Oc1cccc2c1O[C@H]([C@H](C2=C)c3ccccc3)c4ccccc4)=O	5.9
66	O=C1[C@H]([C@](CN1C[C@@H](CC([O-])=O)C)(c2ccccc2)C)c3ccccc3	5.9
67	O[C@H]1[C@](C=2CC[C@@H](C3=COC[C@]1(C32)c4ccccc4)C([O-])=O)(c5ccccc5)C	5.9
68	O=C(O[C@@H]1[C@H](OC[C@H]([C@@H]1Oc2ccccc2)c3ccccc3)OC([O-])=O)C	5.9
69	O=C1[C@H]([C@@](N1CCC([O-])=O)(Cc2ccccc2)c3ccccc3)C	5.9
70	O=C(O[C@H](Cc1ccccc1)c2ccccc2)[C@H](C)C([O-])=O	5.9
71	O[C@H]1[C@@H](O[C@@H]([C@@H]1N(O)CC([O-])=O)c2ccccc2)c3ccccc3	5.9
72	O[C@@H]1[C@H]([C@H](O[C@@H]([C@H]1NC([O-])=O)CO)c2ccccc2)c3ccccc3	5.9
73	[O-]C(SSC[C@@H](Cc1ccccc1)c2ccccc2)=O	5.9
74	[O-]C(O[C@@H]1C[C@@H]([C@@]([C@@H](O1)C)(c2ccccc2)C)c3ccccc3)=O	5.9
75	O=C(NS(=O)(=O)C([O-])=O)[C@]([C@H](c1ccccc1)C)(c2ccccc2)C	5.9
76	O=C(/C=C/[C@](Cc1ccccc1)(c2ccccc2)C)C([O-])=O	5.9
77	[O-]C(=O)C(CC[C@@H](C(c1ccccc1)(C)C)c2ccccc2)=C	5.9
78	[O-]C(O[C@@H]1C[C@@H]([C@@H]([C@@H](O1)C)c2ccccc2)c3ccccc3)=O	5.9
79	O=C(NCCC([O-])=O)[C@](Oc1ccccc1)(c2ccccc2)C	5.9
80	O[C@H]1C[C@@H](O[C@@H]([C@@H]1c2ccccc2)c3ccccc3)ONC([O-])=O	5.9
81	O=C(O[C@@H]1[C@H](O[C@H]([C@H]1c2ccccc2)c3ccccc3)OC([O-])=O)C	5.9
82	[O-]C(=O)CCC[C@@]1(CCCN1c2ccccc2)c3ccccc3	5.8
83	[O-]C(=O)[C@@H](CC(C)C)B1O[C@@]([C@@](O1)(c2ccccc2)C)(c3ccccc3)C	5.8
84	[O-]C(=O)CCC[C@H](Sc1ccccc1)c2ccccc2	5.8
85	[O-]C(OCO[C@H]1C=C([C@H](O1)c2ccccc2)c3ccccc3)=O	5.8
86	[O-]C(=O)CC1=N[C@@](Cc2ccccc2)(CO1)c3ccccc3	5.8

87	[O-]C(O[C@H]1C[C@@](OC)([C@@]([C@@H](O1)C)(c2ccccc2)C)c3ccccc3)=O	5.8
88	O=C([C@H](Oc1ccccc1)CCSC([O-])=O)c2ccccc2	5.8
89	O=C(N[C@H](Cc1ccccc1)c2ccccc2)[C@H](OC([O-])=O)C	5.8
90	OC[C@@H]1[C@H]([C@H](C[C@H]1CC([O-])=O)c2ccccc2)c3ccccc3	5.8
91	O=C(N([C@@H](c1ccccc1)C)Cc2ccccc2)CCC([O-])=O	5.8
92	O=C(O[C@@H]1[C@H](O[C@H]([C@H]1c2ccccc2)c3ccccc3)CC([O-])=O)CC	5.8
93	O=S(=O)(NC[C@](Oc1ccccc1)(c2ccccc2)C)C([O-])=O	5.8
94	O=C1C[C@H]([C@](C(C1)(C)C)(c2ccccc2)/C=C/[C@H](C)C([O-])=O)c3ccccc3	5.8
95	O=S(=O)(N1C[C@@H]([C@@](C2CC2)(C1)c3ccccc3)c4ccccc4)C([O-])=O	5.8
96	[O-][N+](=O)[C@@]1(c2ccccc2)C(OC)=N[C@@H](N=C1c3ccccc3)CC([O-])=O	5.8
97	[O-]C(=O)C[C@H]1CCC(O1)(Cc2ccccc2)Cc3ccccc3	5.8
98	[O-]C(=O)CN1c2ccccc2CN([C@@H](C1)Cc3ccccc3)c4ccccc4	5.8
99	[O-]C(=O)CC1=C[C@@](Nc2ccccc2)(CC1)c3ccccc3	5.8
100	[O-]C(OC=1C=C[C@H]([C@@H](c2ccccc2)C1)c3ccccc3)=O	5.8
101	O=C(/C=C/[C@@H](Cc1ccccc1)c2ccccc2)C([O-])=O	5.8
102	O=C([C@@H]1[C@H](N([C@@H](O1)c2ccccc2)c3ccccc3)CC(C)C)C([O-])=O	5.8
103	O[C@@H]1[C@H]([C@H](C[C@H]1COC([O-])=O)c2ccccc2)c3ccccc3	5.8
104	O=S(=O)(N[C@@H]1C[C@@H]([C@@]1(c2ccccc2)C)c3ccccc3)C([O-])=O	5.8
105	Cl[C@]1([C@@H]([C@@H]1c2ccccc2)COC([O-])=O)c3ccccc3	5.8
106	[O-]C(=O)CCC[C@H](Cc1ccccc1)c2ccccc2	5.8
107	[O-]C(=O)C[C@H]1C[C@H]([C@H](O1)c2ccccc2)c3ccccc3	5.8
108	Oc1ccc([C@@H](Sc2ccccc2)c3ccccc3)cc1C([O-])=O	5.8
109	F[C@@H]1[C@H](O[C@H]([C@H]([C@@H]1O)c2ccccc2)c3ccccc3)OC([O-])=O	5.8
110	[O-]C(=O)[C@H](/C=C/[C@H](Nc1ccccc1)c2ccccc2)C	5.8
111	[O-]C(=O)C[C@@H]1C[C@@H]([C@@H]([N+]1C)c2ccccc2)c3ccccc3	5.7
112	O=C1C=C(N[C@H](Cc2ccccc2)c3ccccc3)[C@@]1(C)C([O-])=O	5.7
113	O=C(N1C[C@H]([C@](C1)(c2ccccc2)C)c3ccccc3)CCC([O-])=O	5.7
114	O=C(OCC([O-])=O)N1[C@H](CO[C@]1(c2ccccc2)C)c3ccccc3	5.7
115	[O-]C(=O)c1cccc([C@@H]([C@@H](c2ccccc2)C)c3ccccc3)c1	5.7
116	[O-]C(=O)CCC[C@](Cc1ccccc1)(c2ccccc2)C	5.7
117	O[C@@H]1[C@@H](O[C@H]([C@@H]1c2ccccc2)CCC([O-])=O)c3ccccc3	5.7
118	[O-]C(=O)C[C@H]1C[C@@H]([C@@H]([C@H](O1)C)c2ccccc2)c3ccccc3	5.7
119	O=S(=O)(NC1[C@]([C@]1(c2ccccc2)C)(c3ccccc3)C)C([O-])=O	5.7
120	[O-]C(=O)C[C@]1([C@@H]([C@H]([C@H](O1)c2ccccc2)c3ccccc3)CC)C	5.7
121	[O-]C(=O)/N=C\C[C@H]1C=C[C@H]([C@H](O1)c2ccccc2)c3ccccc3	5.7
122	[O-]C(SSC[C@@H](Nc1ccccc1)c2ccccc2)=O	5.7
123	[O-]C(=O)c1ccc(o1)[C@@](Cc2ccccc2)(c3ccccc3)C	5.7
124	[O-]C(=O)CCO/N=C(\Cc1ccccc1)c2ccccc2	5.7
125	[O-]C(OC[C@@H]1[C@@H](Oc2ccccc2)[C@@H]([C@H](O1)OC)c3ccccc3)=O	5.7
126	O[C@H]1[C@@H]([C@@H](O[C@]2(C([C@H]([C@H](O2)c3ccccc3)c4ccccc4)(C)C)C)C1)C([O-])=O)C	5.7
127	O=S(=O)(N1CCC[C@H]([C@H](C1)c2ccccc2)c3ccccc3)C([O-])=O	5.7
128	[O-]C(=O)CC[C@@H]1CCC[C@@]1(Cc2ccccc2)c3ccccc3	5.7
129	[O-]C(=O)[C@]1(OC[C@@H](O1)[C@H](Nc2ccccc2)c3ccccc3)C	5.7
130	O=C(O[C@@H]1[C@H](O[C@H]([C@H]1c2ccccc2)c3ccccc3)CC([O-])=O)C(C)C	5.7

131	O=S1(=O)[C@@]([C@@H](N2C(=O)C[C@H]21)c3ccccc3)(c4ccccc4)/C=C/CC([O-])=O	5.7
132	O=C([C@H](N(c1ccccc1)C)CCOC([O-])=O)c2ccccc2	5.7
133	O=C(C#C[C@H](Oc1ccccc1)c2ccccc2)C([O-])=O	5.7
134	[O-]C(SCC[C@H](Cc1ccccc1)c2ccccc2)=O	5.7
135	[O-]C(=O)CO[C@@H]1[C@@H]([C@@H](CO1)c2ccccc2)c3ccccc3	5.7
136	O=C([C@H](c1ccccc1)/C=C/C(=O)C([O-])=O)c2ccccc2	5.7
137	[O-]C(=O)n1cc([C@@H]([C@@H](CC)c2ccccc2)c3ccccc3)cn1	5.7
138	O[C@@H]1[C@@](O[C@H]([C@H]1c2ccccc2)c3ccccc3)(O)C(=O)C([O-])=O	5.7
139	[O-]C(=O)c1c(oc(n1)[C@@H](Cc2ccccc2)c3ccccc3)C	5.7
140	O=S(=O)(N[C@@H]1C[C@@]([C@@]1(c2ccccc2)C)(c3ccccc3)C)C([O-])=O	5.7
141	[O-]C(=O)c1ccnc(N(Cc2ccccc2)Cc3ccccc3)c1	5.7
142	S=C(N(CCCCC([O-])=O)c1ccccc1)c2ccccc2	5.7
143	S=C(SSC([O-])=O)N(Cc1ccccc1)c2ccccc2	5.7
144	O[C@H]1[C@@H](O)[C@@H](O[C@@H]1[C@@H](Sc2ccccc2)c3ccccc3)C([O-])=O	5.7
145	[O-]C(=O)c1cnc2[C@@H](N(CCn12)c3ccccc3)c4ccccc4	5.7
146	O=C1C(CCCC([O-])=O)C(=O)N(N1c2ccccc2)c3ccccc3	5.7
147	O[C@H]1[C@H](O[C@@](Oc2ccccc2)([C@H]1O)c3ccccc3)CC([O-])=O	5.7
148	[O-]C(=O)[C@H]1CCC[C@@H](C1)[C@H](Cc2ccccc2)c3ccccc3	5.7
149	O[C@H]1[C@H]([C@H](O[C@@H]1[C@H](CC)C([O-])=O)c2ccccc2)c3ccccc3	5.7
150	[O-]C(Oc1ccccc1[C@@H](Oc2ccccc2)Cc3ccccc3)=O	5.7
151	O=C1[C@H](O[C@@H]([C@@H](N1C)c2ccccc2)c3ccccc3)CC([O-])=O	5.6
152	O=C(OCC(Cc1ccccc1)(Cc2ccccc2)C)C([O-])=O	5.6
153	OC[C@@H]([C@H]1[C@H](OC)[C@H]([C@H](O1)c2ccccc2)c3ccccc3)C([O-])=O	5.6
154	O=C1[C@@](O[C@@H](CN1CCC([O-])=O)c2ccccc2)(c3ccccc3)C	5.6
155	[O-]C(=O)CCC[C@@H](Oc1ccccc1)Cc2ccccc2	5.6
156	[O-]C(=O)CC#C[C@H](N(c1ccccc1)C)c2ccccc2	5.6
157	O=C(OC[C@H]1C[C@@H]([C@@H](C[C@@H]1CC([O-])=O)c2ccccc2)c3ccccc3)C	5.6
158	O[C@@]1(CN(C[C@]1(c2ccccc2)C)c3c(ccc(n3)C)C([O-])=O)c4ccccc4	5.6
159	[O-]C(=O)c1c(ccc([C@@H](Cc2ccccc2)c3ccccc3)c1)C	5.6
160	O[C@@H]([C@H]1C(=O)C(=C(O1)c2ccccc2)c3ccccc3)CSC([O-])=O	5.6
161	O=C(NS(=O)(=O)C([O-])=O)[C@@]1(CCCN(C1)c2ccccc2)c3ccccc3	5.6
162	I[C@@H]1[C@H](O[C@H]([C@H]([C@H]1O)c2ccccc2)c3ccccc3)OC([O-])=O	5.6
163	O=C1C=2[C@H](CC(=O)NC2C[C@@H]([C@@H]1c3ccccc3)c4ccccc4)C([O-])=O	5.6
164	O=C(OC[C@@H]1[C@@H]([C@H](c2ccccc2)C=CO1)c3ccccc3)C([O-])=O	5.6
165	OC[C@](Cc1ccccc1)(c2ccccc2)c3cccc(c3)C([O-])=O	5.6
166	O=C(N(Cc1ccccc1)Cc2ccccc2)CCC([O-])=O	5.6
167	O=C([C@@](CCOC([O-])=O)(c1ccccc1)C)c2ccccc2	5.6
168	O=C1C(OC([O-])=O)=C[C@@](Cc2ccccc2)(c3ccccc13)c4ccccc4	5.6
169	[O-]C(=O)c1csc([C@@H](Cc2ccccc2)c3ccccc3)c1	5.6
170	O=C1C[C@@]2([C@@]([C@](C1)(CO2)c3ccccc3)(c4ccccc4)/C=C/[C@H](C)C([O-])=O)C	5.6
171	O=C(N[C@](Cc1ccccc1)(c2ccccc2)C)[C@H](C)C([O-])=O	5.6
172	[O-]C(=O)C/C=C(/[C@H](Cc1ccccc1)c2ccccc2)C	5.6
173	O=C(N[C@H](O)C([O-])=O)[C@H]1[C@](C[C@H]1c2ccccc2)(c3ccccc3)C	5.6
174	O[C@]1(CCN(C[C@@]1(c2ccccc2)C)C(=O)C([O-])=O)c3ccccc3	5.6

175	[O-]C(=O)CCO[C@@]1(CCCC[C@@H]1c2ccccc2)c3ccccc3	5.6
176	[O-]C(OC[C@H]1[C@H]([C@@H](c2ccccc2)C=CO1)c3ccccc3)=O	5.6
177	[O-]C(=O)c1ccc(o1)[C@@H](N(C2CCCC2)c3ccccc3)c4ccccc4	5.6
178	[O-]C(=O)CCSCc1cc(n(n1)-c2ccccc2)-c3ccccc3	5.6
179	F[C@@H]1[C@H](O[C@H]([C@H]([C@H]1c2ccccc2)c3ccccc3)C)OC([O-])=O	5.6
180	[O-]C(=O)[C@H]1COC(O[C@@H]1[C@H]2[C@@H](O[C@@](O2)(c3ccccc3)C)c4ccccc4)(C)C	5.6
181	[O-]C(=O)[C@H]([C@@H]1C[C@H]([C@](O1)(c2ccccc2)C)c3ccccc3)C	5.6
182	[O-]C(=O)COC[C@](Cc1ccccc1)(c2ccccc2)C	5.6
183	[O-]C(=O)C[C@@H]1CC[C@@](O1)(Cc2ccccc2)c3ccccc3	5.6
184	[O-]C(=O)[C@H]1CCCN1C2=C([C@@]3([C@H]2c4ccccc4S3)c5ccccc5)c6ccccc6	5.6
185	[O-][n+]1c(cnc2c1[C@](O[C@]2(c3ccccc3)C)(c4ccccc4)C)C([O-])=O	5.6
186	S[C@@H](C[C@H](Cc1ccccc1)c2ccccc2)CC([O-])=O	5.6
187	[O-]C(=O)CSCC[C@H](Sc1ccccc1)c2ccccc2	5.6
188	S=C(NC[C@@H](Cc1ccccc1)c2ccccc2)C([O-])=O	5.6
189	O=C1C[C@H]([C@H](C[C@]12CC(O[C@@H]2C([O-])=O)=O)c3ccccc3)c4ccccc4	5.6
190	Br[C@@]1(C[C@@]1(C(=O)N2C[C@H](O[C@H](C2)C)C([O-])=O)c3ccccc3)c4ccccc4	5.6
191	[O-]C(=O)c1nc(nc(N([C@H](c2ccccc2)C)c3ccccc3)n1)C	5.6
192	O=C(N([C@H](Cc1ccccc1)c2ccccc2)C)CC([O-])=O	5.6
193	[O-]C(=O)CC([C@H]1OC[C@H]([C@H](O1)c2ccccc2)c3ccccc3)(C)C	5.6
194	O=S(=O)(N1CCC[C@](Oc2ccccc2)(C1)c3ccccc3)C([O-])=O	5.6
195	O=C(O[C@@H]([C@@H](c1ccccc1)C)c2ccccc2)CCC([O-])=O	5.6
196	F[C@@]1(C[C@H](N(C1)C(=O)CCC([O-])=O)c2ccccc2)c3ccccc3	5.6
197	O[C@@H]1[C@@H](O[C@@H]([C@H]1OC)[C@@H](Cc2ccccc2)c3ccccc3)C([O-])=O	5.5
198	O=C([C@H](c1ccccc1)C2=N[C@H](SS2)C([O-])=O)c3ccccc3	5.5
199	O=C(O[C@]1([C@H](O[C@@H]([C@@]1(c2ccccc2)C)c3ccccc3)CC([O-])=O)C)C	5.5
200	O=C(N(c1ccccc1)CC(ONC([O-])=O)=O)c2ccccc2	5.5
201	O[C@@H]1C[C@@H](O[C@H]1CN(c2ccccc2)C(=O)c3ccccc3)C([O-])=O	5.5
202	O=C(N1CC[C@]1(c2ccccc2)C(=O)c3ccccc3)C4(CCC4)C([O-])=O	5.5
203	O[C@H]1[C@@H]([C@@H](O[C@@H]1[C@H](C)C([O-])=O)c2ccccc2)c3ccccc3	5.5
204	O=S(=O)(N1C[C@H]([C@](C1)(c2ccccc2)C)c3ccccc3)C([O-])=O	5.5
205	Br[C@@H]1[C@H](O[C@H]([C@H]1c2ccccc2)c3ccccc3)CC([O-])=O	5.5
206	F[C@@]1([C@H](O[C@@]2(CO[C@H]12)CC([O-])=O)c3ccccc3)c4ccccc4	5.5
207	O[C@]1(CO[C@@H]([C@H]1Oc2ccccc2)c3ccccc3)COC([O-])=O	5.5
208	O=C(OCC([O-])=O)N1CC[C@]1(c2ccccc2)C(=O)c3ccccc3	5.5
209	[O-]C(SC([C@H]1OC[C@H]([C@H](O1)c2ccccc2)c3ccccc3)(C)C)=O	5.5
210	O=S(=O)(N1CCC[C@](C1)(Cc2ccccc2)c3ccccc3)C([O-])=O	5.5
211	F[C@@]1(C[C@H](N(C1)C(=O)C(CC([O-])=O)(C)C)c2ccccc2)c3ccccc3	5.5
212	O=C(O[C@H]1[C@@H](O[C@@H]([C@@H]1c2ccccc2)c3ccccc3)CSC([O-])=O)C	5.5
213	[O-]C(OC[C@H]1/C([C@H]([C@H](O1)c2ccccc2)c3ccccc3)=C\C#N)=O	5.5
214	[O-]C(=O)Cc1cnnn1[C@H]2[C@@H](O[C@@H](C2)c3ccccc3)c4ccccc4	5.5
215	O=C(N1CC[C@]1(c2ccccc2)C(=O)c3ccccc3)CCC([O-])=O	5.5
216	Br[C@@H]1[C@H](O[C@H]([C@H]([C@H]1O)c2ccccc2)c3ccccc3)OC([O-])=O	5.5
217	O=C(O[C@@H]([C@@H](c1ccccc1)C)c2ccccc2)CC([O-])=O	5.5
218	O=C(N1C(=NCC1)CC([O-])=O)[C@@H](Cc2ccccc2)c3ccccc3	5.5

219	O=S(=O)(N(C[C@H](Cc1ccccc1)c2ccccc2)C)C([O-])=O	5.5
220	[O-]C(=O)/C=N\O[C@@H]1CN([C@H](C1)c2ccccc2)c3ccccc3	5.5
221	O[C@@H]1[C@@H](O[C@@H](SCC([O-])=O)[C@H]([C@H]1c2ccccc2)c3ccccc3)C	5.5
222	O=C(N[C@@H](C(c1ccccc1)(C)C)c2ccccc2)CC([O-])=O	5.5
223	S=C(N(CCCOC([O-])=O)c1ccccc1)c2ccccc2	5.5
224	[O-]C(=O)c1cccc([C@@H](Cc2ccccc2)c3ccccc3)c1	5.5
225	O=C(OC)[C@@H]([C@H]1C=C[C@H](N(C1)c2ccccc2)c3ccccc3)C([O-])=O	5.5
226	O=C([C@@H](N(c1ccccc1)C)CCSC([O-])=O)c2ccccc2	5.5
227	O=C1[C@H]([C@@](N1c2ccccc2)(c3ccccc3)C(=O)NCCC([O-])=O)C	5.5
228	O[C@@H]([C@]1([C@@H](CC[C@H](O1)CC([O-])=O)C)c2ccccc2)c3ccccc3	5.5
229	O[C@]1([C@H](OC)[C@H](O[C@H]([C@H]1c2ccccc2)c3ccccc3)OC([O-])=O)C	5.5
230	O=S(=O)(N[C@H]1CN(C[C@@H]1c2ccccc2)c3ccccc3)N(C)C([O-])=O	5.5
231	O=C1C[C@]2([C@]([C@@](C1)(CO2)C)(c3ccccc3)/C=C/[C@H](C)C([O-])=O)c4ccccc4	5.5
232	[O-]C(=O)c1cccc(n1)[C@@H](Cc2ccccc2)c3ccccc3	5.5
233	O=C(N1CC[C@@]([N+])([C@@](C1)(c2ccccc2)C)c3ccccc3)C([O-])=O	5.5
234	O[C@H]1[C@H](O)[C@@H]([C@@H](O[C@@H]1S(=O)(=O)C([O-])=O)c2ccccc2)c3ccccc3	5.5
235	O=C(N[C@@H]([C@H](c1ccccc1)C)c2ccccc2)[C@@H](C(C)C)C([O-])=O	5.4
236	O[C@@]1(C[C@H](O[C@@H]([C@H]1c2ccccc2)C)OC([O-])=O)c3ccccc3	5.4
237	O=C([C@]1(CCC[N+](C1)CC(=O)C([O-])=O)c2ccccc2)c3ccccc3	5.4
238	O[C@@H]1C[C@](SC([O-])=O)(O[C@@H]([C@@H]1c2ccccc2)c3ccccc3)C([O-])=O	5.4
239	[O-]C(=O)CCC#C[C@@H](Cc1ccccc1)c2ccccc2	5.4
240	[O-]C(=O)[C@H]([N+][C@H]1C[C@@](O[C@@]1(c2ccccc2)C)(c3ccccc3)C)C	5.4
241	O=C([C@]1([C@@H](C[C@H](OC)[C@H](O1)CC([O-])=O)C)c2ccccc2)c3ccccc3	5.4
242	O=C(NCC([O-])=O)[C@](Cc1ccccc1)(c2ccccc2)C	5.4
243	O[C@@H]1[C@@H](O[C@@H]([C@@H]1c2ccccc2)c3ccccc3)CCC([O-])=O	5.4
244	[O-]C(=O)[C@H]1CC[N+]([C@H]([C@H](c2ccccc2)C)c3ccccc3)C1	5.4
245	FC(F)(F)[C@@](NC(=O)CC([O-])=O)(Nc1ccccc1)c2ccccc2	5.4
246	[O-]C(=O)[C@@]1([C@@H](O1)CC[C@@]2([C@H](O2)c3ccccc3)c4ccccc4)C	5.4
247	[O-]C(=O)[C@H]1CSC(=N1)[C@H](Cc2ccccc2)c3ccccc3	5.4
248	O[C@@H]1[C@H](O[C@H]([C@H]1c2ccccc2)c3ccccc3)[C@@H](OC)OC([O-])=O	5.4
249	O=S(=O)(N1CCO[C@](C1)(c2ccccc2)C(=O)c3ccccc3)C([O-])=O	5.4
250	[O-]C(=O)n1cc(C[C@@H](Cc2ccccc2)c3ccccc3)cn1	5.4
251	[O-]C(=O)[C@H]1CCC[N+]1C[C@H](Cc2ccccc2)c3ccccc3	5.4
252	[O-]C(=O)C/C=C/1CCO[C@@H]([C@@H]1c2ccccc2)c3ccccc3	5.4
253	O=C(OC[C@@]1([C@@H](CC(=C[C@@H]1c2ccccc2)C)C)c3ccccc3)C([O-])=O	5.4
254	[O-]C(=O)[C@H]1C[C@@H](C[N+]([C@H]([C@H](c2ccccc2)C)c3ccccc3)C1)C	5.4
255	[O-]C(=O)N/N=C/1C[C@H]([N+][C@@H]([C@@H]1c2ccccc2)c3ccccc3)c4ccccc4	5.4
256	[O-]C(=O)[C@]1([C@@H](O1)C[C@H](c2ccccc2)C(c3ccccc3)=C)C	5.4
257	[O-]C(=O)C[C@@H]1/C([C@@H]([C@@H](O1)c2ccccc2)c3ccccc3)=C\C#N	5.4
258	O=C([C@@](C[N+]1CCC[C@@H]1C([O-])=O)(c2ccccc2)C)c3ccccc3	5.4
259	[O-]C(=O)[C@]1(Cc2ccccc2C(=N1)[C@H](Cc3ccccc3)c4ccccc4)C	5.4
260	FC(F)(F)c1cc(cc([C@@H](Cc2ccccc2)c3ccccc3)c1)C([O-])=O	5.4
261	[O-]C(S/C=C/[C@@H](Cc1ccccc1)c2ccccc2)=O	5.4
262	O=C(OC[C@]1(Cc2ccccc2CN1c3ccccc3)c4ccccc4)C([O-])=O	5.4

263	[O-]C(=O)[C@H]([C@H]1CC[C@H]([C@H](O1)c2ccccc2)c3ccccc3)CC	5.4
264	[O-]C(SSC[C@@H](Oc1ccccc1)Cc2ccccc2)=O	5.4
265	[O-]C(=O)N1CC[C@@H]1/C(N[C@H](Cc2ccccc2)c3ccccc3)=[N+]\C	5.4
266	[O-]C(O[C@H]1C=C([C@H](C(C1)(C)C)c2ccccc2)c3ccccc3)=O	5.4
267	S=C(SCC([O-])=O)N(Cc1ccccc1)Cc2ccccc2	5.4
268	F[C@@]1([C@](F)(Oc2cccc(c2O1)CC([O-])=O)c3ccccc3)c4ccccc4	5.4
269	O=C(OCC([O-])=O)[C@@]1(CCCN1c2ccccc2)c3ccccc3	5.4
270	[O-]C(=O)CC#C[C@H](Oc1ccccc1)c2ccccc2	5.4
271	[O-]C(=O)CCC[N+](Cc1ccccc1)Cc2ccccc2	5.4
272	Fc1cc(cc([C@@H](Cc2ccccc2)c3ccccc3)c1)C([O-])=O	5.4
273	O=C(N[C@@]1(CCCC[C@H]1c2ccccc2)c3ccccc3)CC([O-])=O	5.4
274	O[C@H]1[C@@H]([C@@H](O[C@@H]1CCCC([O-])=O)c2ccccc2)c3ccccc3	5.4
275	O[C@H]([C@@H](NC(SC([O-])=O)=O)c1ccccc1)c2ccccc2	5.4
276	O[C@H]1[C@H](O[C@H]([C@H]1c2ccccc2)c3ccccc3)/C=N\C([O-])=O	5.4
277	[O-]C(=O)C[C@H]1C=C([C@H](S1)c2ccccc2)c3ccccc3	5.4
278	O[C@@H]1[C@H](OCO[C@@H]1[C@@H](Cc2ccccc2)c3ccccc3)C([O-])=O	5.4
279	O[C@H]1[C@@H](O[C@@H](SCC([O-])=O)[C@@H]1c2ccccc2)c3ccccc3	5.4
280	[O-]C(=O)C[C@@H]1C[N+]([C@@H](CO1)c2ccccc2)Cc3ccccc3	5.4
281	O=C([C@@H](SC1=NN1C([O-])=O)c2ccccc2)c3ccccc3	5.4
282	[O-]C(=O)c1nccc(N(Cc2ccccc2)c3ccccc3)n1	5.4
283	[O-]C(=O)C/C=C/[C@H](Cc1ccccc1)c2ccccc2	5.4
284	[O-]C(=O)c1cnc([nH]1)[C@@H](Cc2ccccc2)c3ccccc3	5.4
285	[O-]C(=O)[C@@]1(C[N+]([C@@H](Cc2ccccc2)c3ccccc3)CCO1)C	5.4
286	O=[S@](C[C@H](Nc1ccccc1)c2ccccc2)CC([O-])=O	5.4
287	O=C(OC[C@]1([C@@H](C=C(C[C@H]1c2ccccc2)C)C)c3ccccc3)C([O-])=O	5.4
288	O=C(NC([O-])=O)[C@H]1CCC[N+]1[C@@H]([C@@H](c2ccccc2)C)c3ccccc3	5.4
289	[O-]C(=O)CCSC([C@@H](Nc1ccccc1)c2ccccc2)(C)C	5.4
290	O=C(N(C[C@H]1CCC[N+]1CC([O-])=O)c2ccccc2)c3ccccc3	5.4
291	[O-]C(=O)CCN1c2ccccc2C(=C[C@@H]([C@H]1C)c3ccccc3)c4ccccc4	5.4
292	[O-]C(=O)CCC[C@@](Sc1ccccc1)(c2ccccc2)C#N	5.4
293	O=C1[C@@H](O[C@@H](C=C1C[N+]2CCCC[C@@H]2C([O-])=O)c3ccccc3)c4ccccc4	5.4
294	O=C1[C@@H](C[C@H](O1)[C@@H](Cc2ccccc2)c3ccccc3)C([O-])=O	5.4
295	[O-]C(=O)C[C@@H]1C=C([C@@H](C[C@H]1C(C)C)c2ccccc2)c3ccccc3	5.4
296	Clc1ccc([C@H](c2ccccc2)/C(=N/N)c3ccccc3)cc1C([O-])=O	5.4
297	FC(F)(F)[C@](Cc1ccccc1)(c2ccccc2)/C=C/OC([O-])=O	5.4
298	O=C1[C@@H]([C@@H](Sc2ccccc2N1CC([O-])=O)c3ccccc3)c4ccccc4	5.4
299	O=C(O[C@@H]1C[C@H](O[C@H]([C@H]1c2ccccc2)c3ccccc3)OC([O-])=O)C	5.4
300	O=C([C@@](NC(=O)[C@H](C)C([O-])=O)(c1ccccc1)C)c2ccccc2	5.3
301	[O-]C(=O)C1(OC[C@H](Cc2ccccc2)c3ccccc3)CCCCC1	5.3
302	O=C([C@@H](Cc1ccccc1)c2ccccc2)/C=C/C([O-])=O	5.3
303	O[C@H]1C[C@](O[C@@H]([C@@H]1c2ccccc2)c3ccccc3)(OC)C(=O)C([O-])=O	5.3
304	O[C@]1([C@@H](O[C@@H]([C@H]1O)COC([O-])=O)c2ccccc2)c3ccccc3	5.3
305	F[C@]1([C@@H](O[C@@H]([C@H]1O)COC([O-])=O)c2ccccc2)c3ccccc3	5.3
306	O=C(N[C@](Cc1ccccc1)(c2ccccc2)C)CC([O-])=O	5.3

307	[O-]C(OCC[C@@](Cc1ccccc1)(c2ccccc2)C)=O	5.3
308	FC(F)(CC[C@H](NC(=O)c1ccccc1)c2ccccc2)C([O-])=O	5.3
309	[O-]C(=O)Cn1cncc1Cn2cc(c(c2)-c3ccccc3)-c4ccccc4	5.3
310	O[C@H]1[C@@H](O)C(=C[C@]1(Cc2ccccc2)c3ccccc3)CC([O-])=O	5.3
311	Fc1ccc([C@@](O)(Cc2ccccc2)c3ccccc3)cc1C([O-])=O	5.3
312	[O-]C(O[C@@]1(OC)C=C[C@](OC)(C(=C1)c2ccccc2)c3ccccc3)=O	5.3
313	[O-]C(=O)c1noc(n1)[C@@](Cc2ccccc2)(c3ccccc3)C	5.3
314	O=C1[C@@H]([C@@H](Sc2ccccc2N1CCC([O-])=O)c3ccccc3)c4ccccc4	5.3
315	O=C1C=C([C@@](C(C1)(C)C)(/C=C/[C@@H](C)C([O-])=O)c2ccccc2)c3ccccc3	5.3
316	[O-]C(=O)COC[C@H](N(CC)c1ccccc1)c2ccccc2	5.3
317	[O-]C(=O)C1C[N+](C1)C[C@H](Cc2ccccc2)c3ccccc3	5.3
318	[O-]C(=O)CO[C@H]([C@H](Cc1ccccc1)c2ccccc2)C	5.3
319	[O-]C(=O)C[N+][C@@H]1C[C@@H]([C@@]1(c2ccccc2)C)c3ccccc3	5.3
320	OC[C@@H]1C[N+]([C@H](Cc2ccccc2)c3ccccc3)C[C@H](O1)C([O-])=O	5.3
321	O=C(NS(=O)(=O)C([O-])=O)[C@](Cc1ccccc1)(c2ccccc2)C	5.3
322	[O-]C(=O)[C@@H]1CC(=NO1)[C@@H](Cc2ccccc2)c3ccccc3	5.3
323	[O-]C(=O)CO/N=C\Cc1c(c(ns1)-c2ccccc2)-c3ccccc3	5.3
324	O[C@H]([C@H]1[C@H](OC)[C@H]([C@H](O1)c2ccccc2)c3ccccc3)CC([O-])=O	5.3
325	O=C([C@]1(CC[N+]1CCC([O-])=O)c2ccccc2)c3ccccc3	5.3
326	O=S(=O)(/C=C/[C@H](Cc1ccccc1)c2ccccc2)C([O-])=O	5.3
327	[O-]C(=O)CCO[C@@H](Cc1ccccc1)c2ccccc2	5.3
328	F[C@@]1([C@H](O[C@](F)([C@@H]1O)COC([O-])=O)c2ccccc2)c3ccccc3	5.3
329	[O-]/[N+](=C\[C@H](Cc1ccccc1)c2ccccc2)CC([O-])=O	5.3
330	O[C@H]1C[C@](O[C@@H]([C@@H]1c2ccccc2)c3ccccc3)(O)[C@@H](O)C([O-])=O	5.3
331	O[C@H]1[C@@H](O)C[C@@H](O[C@H]1[C@H](Cc2ccccc2)c3ccccc3)C([O-])=O	5.3
332	[O-]C(=O)[C@@H]1C[N+]([C@H](Cc2ccccc2)c3ccccc3)C[C@H](O1)C	5.3
333	O[C@@H]1[C@H](O[C@]([C@H]1c2ccccc2)(c3ccccc3)C)[C@@H](C)C([O-])=O	5.3
334	[O-]C(=O)C[C@]1(CC[C@H]([C@](O1)(c2ccccc2)C)c3ccccc3)C	5.3
335	O=C(N(CCCCC([O-])=O)c1ccccc1)c2ccccc2	5.3
336	S=C([C@H](c1cc(ccc1OC)C([O-])=O)c2ccccc2)c3ccccc3	5.3
337	[O-]C(=O)[C@@]1(O[C@H]([C@H](c2ccccc2)C(c3ccccc3)=C)CO1)C	5.3
338	O=C(N(CCOCC([O-])=O)c1ccccc1)c2ccccc2	5.3
339	O=C1[C@@H](N(C(=O)[C@H](S(=O)(=O)C([O-])=O)N1C)c2ccccc2)c3ccccc3	5.2
340	O=C(N1[C@H](CCC1)C([O-])=O)C[C@H](Cc2ccccc2)c3ccccc3	5.2
341	O[C@@]1([C@H](O)[C@H](O[C@]1(c2ccccc2)C#N)CC([O-])=O)c3ccccc3	5.2
342	[O-]C(O[C@@H]1C[C@@H]([N+](C)C)[C@@H]([C@@H](O1)c2ccccc2)c3ccccc3)=O	5.2
343	[O-]C(=O)CSC[C@H](Cc1ccccc1)c2ccccc2	5.2
344	[O-]C(=O)c1cccc(CS/C(c2ccccc2)=C/c3ccccc3)c1	5.2
345	OCC[C@]1(CC[C@@H](C[C@@H]1c2ccccc2)CC([O-])=O)c3ccccc3	5.2
346	[O-]C(=O)CCC[C@@](Nc1ccccc1)(c2ccccc2)C	5.2
347	[O-]C(=O)CC[N+](C1CC1)[C@H](Cc2ccccc2)c3ccccc3	5.2
348	[O-]C(=O)N1CC[C@@H]1/C(=[N+]/[C@H](Cc2ccccc2)c3ccccc3)N	5.2
349	O=C(N[C@@H]1C[C@H](O[C@H]([C@H]1c2ccccc2)c3ccccc3)OC([O-])=O)C	5.2
350	O[C@@H]1[C@H](O[C@]([C@H]1c2ccccc2)(c3ccccc3)CO)CC([O-])=O	5.2

351	O=C([C@H](c1ccccc1)/C=C/CC([O-])=O)c2ccccc2	5.2
352	[O-]C(OCc1cnnn1[C@H]2[C@@H](O[C@@H](C2)c3ccccc3)c4ccccc4)=O	5.2
353	[O-]C(=O)C(SC[C@H](Nc1ccccc1)c2ccccc2)(C)C	5.2
354	O=C(OCC([O-])=O)CC[C@@H](Nc1ccccc1)c2ccccc2	5.2
355	[O-]C(=O)[C@@H]1[C@@H](C[C@@H](Nc2ccccc2)c3ccccc3)c4ccccc4N1	5.2
356	O[C@H]1[C@H](O)[C@@H]([C@@H]([C@@H](O1)OCC([O-])=O)c2ccccc2)c3ccccc3	5.2
357	[O-]C(=O)CCN1c2ccccc2C(=C[C@H]([C@H]1c3ccccc3)c4ccccc4)C	5.2
358	[O-]C(=O)COC[C@H](N(c1ccccc1)C)c2ccccc2	5.2
359	O=C(NN(C)C([O-])=O)[C@@](Oc1ccccc1)(CC)c2ccccc2	5.2
360	O=C([C@@]([N+]CCOC([O-])=O)(c1ccccc1)C)c2ccccc2	5.2
361	O=C1CCc2cc(cc([C@@H](Cc3ccccc3)c4ccccc4)c2N1)C([O-])=O	5.2
362	[O-]C(=O)[C@@H](SC[C@H](Nc1ccccc1)c2ccccc2)C	5.2
363	[O-]C(=O)c1nc(no1)[C@@H](Cc2ccccc2)c3ccccc3	5.2
364	O=S(=O)(NC[C@@](Cc1ccccc1)(c2ccccc2)C)C([O-])=O	5.2
365	[O-]C(=O)CC#C[C@]1(CCCC[C@H]1c2ccccc2)c3ccccc3	5.2
366	[O-]C(=O)C[N+](C[C@](Cc1ccccc1)(c2ccccc2)C)C	5.2
367	O=C(N1CC(C1)C([O-])=O)[C@]2(C[C@@]2(c3ccccc3)C)c4ccccc4	5.2
368	O[C@@]1([C@H](O)[C@H](O[C@H]1c2ccccc2)CC([O-])=O)c3ccccc3	5.2
369	[O-]C(O[C@@H]1C[C@@H]([N+]2CCOCC2)[C@@H]([C@@H](O1)c3ccccc3)c4ccccc4)=O	5.2
370	O=C1[C@@H](SCCC([O-])=O)[C@H](N1c2ccccc2)c3ccccc3	5.2
371	O=C(SC([O-])=O)N[C@@H](Cc1ccccc1)c2ccccc2	5.2
372	O=C(N1C[C@H](C[C@H]1c2ccccc2)c3ccccc3)N(CC([O-])=O)C	5.2
373	O=C([C@@H]1[C@H](O[C@](O1)(C)C([O-])=O)C)[C@@H](Oc2ccccc2)c3ccccc3	5.2
374	O[C@@H]([C@]1([C@@H](CC[C@H](O1)[C@H](C)C([O-])=O)C)c2ccccc2)c3ccccc3	5.2
375	O=C1C=C([C@@]([C@](C1)(c2ccccc2)C)(c3ccccc3)/C=C/[C@H](C)C([O-])=O)C	5.2
376	O=C(OC[C@@H]1[C@@H](OC([O-])=O)C=C([C@H](O1)c2ccccc2)c3ccccc3)C	5.2
377	[O-]C(=O)COC[C@H](Cc1ccccc1)c2ccccc2	5.2
378	O=C([C@]1(CCC=C[C@H]1c2ccccc2)c3ccccc3)/C=C/C([O-])=O	5.2
379	[O-]C(=O)CCCN([C@@H](c1ccccc1)C)c2ccccc2	5.2
380	[O-]C(=O)c1cc(on1)[C@](Sc2ccccc2)(SC)c3ccccc3	5.2
381	O=C(N(C)C([O-])=O)CC[C@@H](Cc1ccccc1)c2ccccc2	5.1
382	[O-]C(=O)CN1c2ccc(cc2CN([C@@H](C1)c3ccccc3)c4ccccc4)C#N	5.1
383	O[C@@H]([C@@H](c1ccccc1)c2nc(cs2)C([O-])=O)c3ccccc3	5.1
384	O[C@@]1([C@H](O)[C@H](O[C@H]1c2ccccc2)C(=O)C([O-])=O)c3ccccc3	5.1
385	O=C([C@@H](NOC(=O)C([O-])=O)c1ccccc1)c2ccccc2	5.1
386	[O-]C(=O)[C@H]1COC(=N1)[C@@H](Cc2ccccc2)c3ccccc3	5.1
387	O[C@](C1(CCCC1)c2ccccc2)(c3ccccc3)C#CCC([O-])=O	5.1
388	[O-]C(=O)[C@@H]1/C(CCC1)=C/[C@@H](Cc2ccccc2)c3ccccc3	5.1
389	Clc1cc(cc([C@@H](Oc2ccccc2)c3ccccc3)c1)C([O-])=O	5.1
390	S=C(SC[C@@](O)(Cc1ccccc1)c2ccccc2)C([O-])=O	5.1
391	[O-]C(O/N=C(/[C@@H](Cc1ccccc1)c2ccccc2)CC)=O	5.1
392	O=C([C@@](NC(=O)CC([O-])=O)(c1ccccc1)C)c2ccccc2	5.1
393	[O-]C(=O)[C@H](CC/C=C(\Cc1ccccc1)c2ccccc2)C	5.1
394	O=C([C@@H]1[C@@H](OC(=O)C)[C@@H]([C@@H](O1)c2ccccc2)c3ccccc3)C([O-])=O	5.1

395	[O-]C(=O)CO[C@@H]1[C@H]2OC[C@H](O2)[C@@H]([C@@H]1c3ccccc3)c4ccccc4	5.1
396	O[C@H]1[C@@H](O)[C@H](O[C@@]1(c2ccccc2)C(=O)c3ccccc3)CC([O-])=O	5.1
397	[O-]C(=O)c1noc(n1)C[C@@H](Cc2ccccc2)c3ccccc3	5.1
398	[O-]C(=O)[C@]1(C[N+]=C(N1)[C@H](Cc2ccccc2)c3ccccc3)C	5.1
399	Fc1ccc([C@H]([C@@H](Cc2ccccc2)c3ccccc3)C)cc1C([O-])=O	5.1
400	S=C1N(N=C(O1)C([O-])=O)[C@@H](Nc2ccccc2)c3ccccc3	5.1
401	O=C([C@]1(CCCN1c2ccccc2)c3ccccc3)CCC([O-])=O	5.1
402	O=S(=O)(N(c1ccccc1)C(=O)/C=C/C([O-])=O)c2ccccc2	5.1
403	[O-]C(=O)CC[N+][C@@](Cc1ccccc1)(CC)c2ccccc2	5.1
404	O=C([C@@H]([N+]1C[C@H](O[C@@H](C1)C)C([O-])=O)c2ccccc2)c3ccccc3	5.1
405	[O-]C(=O)Nc1cccc2c1C[C@H]([C@H](C2)c3ccccc3)c4ccccc4	5.1
406	O=C1[C@H]([N+][C@@](N1Cc2ccccc2)(CC)c3ccccc3)CC([O-])=O	5.1
407	[O-]C(SCC[C@@](Cc1ccccc1)(c2ccccc2)C)=O	5.1
408	O=C(O[C@@H]([C@@H](C=C(C)C)c1ccccc1)c2ccccc2)CC([O-])=O	5.1
409	[O-]C(=O)CCCN(Cc1ccccc1)c2ccccc2	5.1
410	[O-]C(=O)[C@H]1CC[N+]([C@@H]([C@H](CC)c2ccccc2)c3ccccc3)C1	5.1
411	[O-]C(=O)CCSC1=[N+][C@@H]([C@@H](N1)c2ccccc2)c3ccccc3	5.0
412	[O-]C(=O)c1cc(ns1)[C@@H](Cc2ccccc2)c3ccccc3	5.0
413	[O-]C(=O)c1ccnc(N([C@H](c2ccccc2)C)c3ccccc3)c1	5.0
414	[O-]C(=O)CCC[N+]1CC(=C(N(C1)C)c2ccccc2)c3ccccc3	5.0
415	O=[S@](N(CCOC([O-])=O)c1ccccc1)c2ccccc2	5.0
416	[O-]C(=O)C[N+]C[C@](Cc1ccccc1)(c2ccccc2)C	5.0
417	[O-]C(=O)CCCN(c1ccccc1)C(=C(C)C)c2ccccc2	5.0
418	[O-]C(=O)C[N+]1CCOC[C@](C1)(Cc2ccccc2)c3ccccc3	5.0
419	O=C1C[C@](C(=NN1CC([O-])=O)c2ccccc2)(c3ccccc3)C	5.0
420	O=C1[C@H](C[C@](C[C@H]1[C@@H](Cc2ccccc2)c3ccccc3)(C)C([O-])=O)C	5.0
421	O=C([C@@H](C[N+](CC)CC([O-])=O)c1ccccc1)c2ccccc2	5.0
422	[O-]C(=O)N(CC[N+]1CC[C@@H]([C@@H](C1)c2ccccc2)c3ccccc3)C	5.0
423	O=C1[C@H](OC(=O)C)[C@H](O[C@H]([C@H]1c2ccccc2)c3ccccc3)OC([O-])=O	5.0
424	O=C(N(C1(CCC1)c2ccccc2)c3ccccc3)/C=C/C([O-])=O	5.0
425	O=C1CC[C@@H](C[C@H]1[C@@H](Cc2ccccc2)c3ccccc3)C([O-])=O	5.0
426	[O-]C(=O)C[N+]CC(Cc1ccccc1)Cc2ccccc2	5.0
427	O[C@H]1[C@@H]([N+][C@H]([C@@H]1c2ccccc2)CSC([O-])=O)c3ccccc3	5.0
428	O[C@H]1[C@@H]([N+])[C@@H](O[C@@H]([C@@H]1c2ccccc2)c3ccccc3)OCC([O-])=O	5.0
429	O=C([C@@H]([N+]1C[C@@](O[C@@H](C1)C)(C)C([O-])=O)c2ccccc2)c3ccccc3	5.0
430	O=C(NCC([O-])=O)[C@](NC(=O)C)(Cc1ccccc1)c2ccccc2	5.0
431	O[C@H]1C[C@@H]([N+][C@@H]([C@@H]1c2ccccc2)c3ccccc3)CCC([O-])=O	5.0
432	O=C([C@@](C[N+](CC([O-])=O)C)(c1ccccc1)C)c2ccccc2	5.0
433	[O-]C(=O)[C@@H]1C[N+]([C@@H]([C@@H](c2ccccc2)C)c3ccccc3)[C@@H](CO1)C	5.0
434	[O-]C(=O)CC[C@@H]1[C@@](O1)(Cc2ccccc2)c3ccccc3	5.0
435	O=C(N(CCSSC([O-])=O)c1ccccc1)c2ccccc2	5.0
436	[O-]C(=O)[C@H]([C@]1(CC[C@H]([C@](O1)(c2ccccc2)C)c3ccccc3)C)C	4.9
437	[O-]C(=O)CC[N+]1Cc2ccccc2N(C[C@@H]1c3ccccc3)c4ccccc4	4.9
438	[O-]C(=O)c1cccc(N([C@@H](CC)c2ccccc2)c3ccccc3)c1	4.9

439	O=C1N[C@H]2c3cccc(OC([O-])=O)c3O[C@@](N1c4ccccc4)(C2)c5ccccc5	4.9
440	O[C@H]1[C@H](O[C@@H]([C@@H]([C@@H]1[N+]CC([O-])=O)c2ccccc2)c3ccccc3)C	4.9
441	[O-]C(=O)[C@]1(ON=C(O1)[C@@H](Cc2ccccc2)c3ccccc3)C	4.9
442	O=C([C@@](C[N+]1[C@H](CCC[C@H]1C)C([O-])=O)(c2ccccc2)C)c3ccccc3	4.9
443	O=C([C@@]([N+]CCC([O-])=O)(c1ccccc1)C)c2ccccc2	4.9
444	O=C([C@H](c1cc(cc(c1OC)C)C([O-])=O)c2ccccc2)c3ccccc3	4.9
445	OCc1ccc(cc1N(Cc2ccccc2)c3ccccc3)C([O-])=O	4.9
446	O=C(NCC([O-])=O)[C@]1(COC[C@@H]1c2ccccc2)c3ccccc3	4.9
447	Clc1cc(cc(N(Cc2ccccc2)c3ccccc3)c1)C([O-])=O	4.9
448	[O-]C(=O)c1nc(no1)CSc2nnc(n2-c3ccccc3)-c4ccccc4	4.9
449	O=C(N[C@@H]1C[C@H](O[C@H]([C@H]1c2ccccc2)c3ccccc3)OC([O-])=O)C[N+]	4.9
450	O=C([C@]1(C[C@H]1C[N+]CC([O-])=O)c2ccccc2)c3ccccc3	4.9
451	[O-]C(=O)NCc1cccnc1N(Cc2ccccc2)c3ccccc3	4.9
452	Cl[C@@]1(C[C@@]1(C(=O)N2CCC[C@@H](C2)C([O-])=O)c3ccccc3)c4ccccc4	4.8
453	O=C(NCC([O-])=O)[C@@H](N(C1CC1)c2ccccc2)c3ccccc3	4.8
454	O=C(NC[C@H]1CC[C@H]([C@@H](O1)c2ccccc2)c3ccccc3)C([O-])=O	4.8
455	[O-]C(=O)C[N+][C@H]1C=C[C@H]([C@H]1c2ccccc2)c3ccccc3	4.8
456	SC1=[N+][C@@H](C[C@H](N1)[C@@H](c2ccccc2)C(=O)c3ccccc3)C([O-])=O	4.8
457	O[C@@H](/C(=C\CCC([O-])=O)c1ccccc1)c2ccccc2	4.8
458	O=C1N(C[C@@](O1)(C)C([O-])=O)[C@@H](Cc2ccccc2)c3ccccc3	4.8
459	[O-]C(=O)c1cccc([C@@H]([C@H]([N+]C)c2ccccc2)c3ccccc3)c1	4.8
460	[O-]C(=O)C[N+][C@H]1CC[C@H]([C@H]1c2ccccc2)c3ccccc3	4.8
461	[O-]C(=O)[C@H](C(C)C)B1O[C@]([C@](O1)(c2ccccc2)C)(c3ccccc3)C	4.8
462	[O-]C(=O)[C@H]1[C@H](C[N+](C1)[C@@H](Cc2ccccc2)c3ccccc3)C	4.8
463	O=C(N[C@@H](C)C([O-])=O)[C@]1(CCN1c2ccccc2)c3ccccc3	4.8
464	[O-]C(=O)c1nc(N(Cc2ccccc2)c3ccccc3)c4c(n1)CC[N+](CC4)C	4.8
465	O=C(N1C[C@@H]2CC(=C([C@@H]([N+]2)C1)c3ccccc3)c4ccccc4)CC([O-])=O	4.7
466	O=C(N/N=C(\[C@H](c1ccccc1)c2ccco2)c3ccccc3)C([O-])=O	4.7
467	[O-]C(=O)CC[N+]([C@@H](Cc1ccccc1)c2ccccc2)C	4.7
468	O[C@@H]1C=C[C@@H]([N+]CC([O-])=O)[C@H]([C@H]1c2ccccc2)c3ccccc3	4.7
469	O=C1[C@@H]([C@@H](CN1CCC([O-])=O)c2ccccc2)c3ccccc3	4.7
470	[O-]C(=O)c1cccc(C([C@H]2C[N+][C@@H]([C@H]2c3ccccc3)c4ccccc4)=C)c1	4.7
471	[O-]C(=O)c1ccc(c(N(Cc2ccccc2)c3ccccc3)n1)C[N+]	4.7
472	Clc1cc(cc([C@@]2([C@H]([N+]C(CO2)(C)C)c3ccccc3)c4ccccc4)c1)C([O-])=O	4.7
473	[O-]C(=O)CNC1=[N+][C@H]([C@H]([C@H](N1CC)C)c2ccccc2)c3ccccc3	4.7
474	O=C1[C@H]([C@@H]([C@H]([C@@H](O1)[C@H]2CO[C@](O2)(C)C([O-])=O)C)c3ccccc3)c4ccccc4	4.7
475	[O-]C(=O)C[N+]1CCC[C@](C1)(Cc2ccccc2)c3ccccc3	4.7
476	[O-]C(=O)c1nc(no1)[C@]2(CCCC[C@H]2c3ccccc3)c4ccccc4	4.7
477	[O-]C(SC[C@@H]1CO[C@](O1)(Cc2ccccc2)c3ccccc3)=O	4.7
478	O=C([C@@H]([N+]1C[C@H](CC1)C([O-])=O)c2ccccc2)c3ccccc3	4.7
479	[O-]C(=O)[C@H]1CC[N+](C1)[C@@H](Cc2ccccc2)c3ccccc3	4.7
480	O=C([C@]([N+]C)(c1ccccc1)CSCC([O-])=O)c2ccccc2	4.7
481	O[C@]1([C@@H](O[C@@H]([C@H]1O)CSC([O-])=O)c2ccccc2)c3ccccc3	4.7
482	O=C([C@]([N+]CCC([O-])=O)(CC)c1ccccc1)c2ccccc2	4.7

483	O[C@@]1(C[N+](CC[C@H]1c2ccccc2)CC([O-])=O)c3ccccc3	4.7
484	O=C1[C@@H]([C@@](CN1[C@H](CC([O-])=O)C)(c2ccccc2)C)c3ccccc3	4.6
485	[O-]C(=O)CSC[C@@]([N+])(Cc1ccccc1)c2ccccc2	4.6
486	O=C1[C@@](CCCN1CC([O-])=O)(Cc2ccccc2)c3ccccc3	4.6
487	O=C(OC([O-])=O)C[C@@](Cc1ccccc1)(c2ccccc2)C(OC)=O	4.6
488	O=C(N[C@@H](Cc1ccccc1)c2ccccc2)N(CC([O-])=O)C	4.6
489	[O-]C(=O)[C@H]1CS[C@@H]([N+]1)[C@@H](Cc2ccccc2)c3ccccc3	4.6
490	[O-]C(=O)[C@@]1(C[N+]([C@@H](Cc2ccccc2)c3ccccc3)CCN1C)C	4.6
491	[O-]C(=O)CC[N+]C1[C@@]([C@@]1(c2ccccc2)C)(c3ccccc3)C	4.6
492	[O-]C(=O)[C@@H]([N+]C[C@@](Cc1ccccc1)(c2ccccc2)C)C	4.5
493	O=C1[C@@](CCCCN1CC([O-])=O)(Cc2ccccc2)c3ccccc3	4.5
494	O=C(NC(=O)C([O-])=O)CSc1nc(c(s1)-c2ccccc2)-c3ccccc3	4.5
495	O=C(C[N+]1Cc2ccccc2N(C[C@@H]1c3ccccc3)c4ccccc4)C([O-])=O	4.5
496	[O-]C(=O)C[N+][C@@H]1CCC[C@]1(Cc2ccccc2)c3ccccc3	4.4
497	[O-]C(=O)C/C=N/N(Cc1ccccc1)c2ccccc2	4.4
498	O=C(NCC([O-])=O)[C@@]1(c2ccccc2)C=CCN1c3ccccc3	4.3
499	[O-]C(=O)[C@@]1(C[C@@H](N(Cc2ccccc2)c3ccccc3)CC[N+]1C)C	4.3
500	O=C([C@H]1CCC[N+]1C[C@H](Cc2ccccc2)c3ccccc3)C([O-])=O	4.2